

ExoMol line lists – LXIX. A ro-vibrational line list for the NO⁺ molecular ion

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ABSTRACT

The nitrosyl ion, NO⁺, is the dominant molecular ion in the Earth’s ionosphere and has been detected in the atmospheres of other Solar system planets. A comprehensive and accurate rotation-vibration line list, the NOPE (N, O, Plus, and the lead author’s first initial) line list, for the X¹Σ⁺ (ground electronic) state of ¹⁴N¹⁶O⁺ is presented and tested against empirical data. This line list is applicable up to temperatures of 5000 K. The NOPE line list contains a total of 3881 rovibrational states with 54 434 transitions between them. Vibrational states up to $v = 41$ are considered for rotational states with $J \leq 100$. The NOPE line list is available from the ExoMol data base at www.exomol.com.

Key words: molecular data – opacity – planets and satellites: atmospheres – stars: atmospheres – ISM: molecules.

1 INTRODUCTION

The closed shell nitrosyl ion, NO⁺, is isoelectronic with the CO molecule and has no unpaired valence electrons (J.-P. Zhang et al. 2011). The electronic ground state is the X¹Σ⁺ state, which is the only electronic state studied in this work. NO⁺ is the dominant molecular ion in the Earth’s ionosphere, the upper portion of the Earth’s atmosphere, which is defined by its low density and the presence of charged particles (J. K. Hargreaves 1992; R. F. Pfaff 2012). In the ionosphere NO⁺ is not the product of neutral NO ionization, but arises following the photoionization of molecular nitrogen (R. F. Pfaff 2012). Due to its formation from oxygen, NO⁺ is also an indirect consequence of the presence of life on Earth – the Earth’s secondary atmosphere only contains oxygen at a high percentage because of the presence of oxygenic photosynthesis on Earth (H. Lammer et al. 2018). However, in this context it should be noted that NO⁺ is an important species in the ionospheres of both Venus (K. M. Ambili, S. S. Babu & R. K. Choudhary 2019; K. M. Ambili et al. 2022) and Mars (J. Y. Chaufray et al. 2014; Y. T. Cao et al. 2019). This makes it a particularly interesting target for exoplanet spectroscopy studies as the field moves toward characterizing atmospheres of planets. Additionally, J. Cernicharo et al. (2014) reported a tentative detection of NO⁺ towards the cold dense core Barnard 1-b through its $J = 2 - 1$ pure rotational transition.

The HITRAN data base (I. E. Gordon et al. 2026) contains an infrared line list for the NO⁺ ion, considering transitions within its electronic ground state, for the most common ¹⁴N¹⁶O⁺ isotopologue only. It is this spectral region and species that are the subject of this work. However, HITRAN spectroscopic data are suitable for modelling Earth-like temperatures at 296 K. The highest wavenumber feature in the HITRAN data set corresponds to the first vibrational transition of NO⁺ (L. S. Rothman et al.

2009) ($\Delta v = 1$). However, on exoplanets at high temperatures, many higher vibrational states will be occupied. Therefore, an updated NO⁺ line list is necessary, one that extends to higher wavenumber features than the HITRAN line list, where more features become prominent at higher temperatures. This new line list is presented as part of the ExoMol project (J. Tennyson & S. N. Yurchenko 2012; J. Tennyson et al. 2024). While there have been laboratory and other observations of high resolution spectra of NO⁺, thus far there have been no experimental determinations of transition intensities. Therefore the transition intensities and associated Einstein A coefficients rely on theoretical dipole moments obtained from *ab initio* calculations. We review the status of these below.

For the generation of this line list, three main types of input data for the ground state of NO⁺ were necessary: observed transitions of the molecule, a calculated potential energy curve (PEC), and a calculated dipole moment curve (DMC). These three data sets were collected during a comprehensive review of the literature. The observed transitions are input into the measured active rotational-vibrational energy levels procedure (MARVEL; T. Furtenbacher, A. G. Császár & J. Tennyson 2007), which calculates empirical state energies. PECs are input into DUO (S. N. Yurchenko et al. 2016), which solves the nuclear-motion Schrödinger equation for rovibrational energies and wavefunctions, where the PEC is refined based on empirical (MARVEL) energy levels or transition wavenumbers. DUO can also calculate transition intensities using a DMC and wavefunctions generated using a given PEC. These steps are detailed in the following sections.

2 INPUT DATA

2.1 Observational data

To prepare for input into MARVEL all ro-vibrational transitions of NO⁺ within the ground electronic state available in the liter-

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Table 1. Summary of Earth, laboratory, and interstellar observations of NO⁺, excluding those of M. López-Puertas et al. (2006). Hyperfine components corresponding to the same pair of upper and lower rotational states were averaged to a single pure rotational transition. ‘A/V’ is the number of actual lines in the source/number of lines validated by MARVEL.

Source	A/V	Uncertainty (cm ⁻¹)	Frequency (cm ⁻¹)	Transition			
				v'	J'	v''	J''
F. Alberti & A. E. Douglas (1975)	1/1	0.001	3.976	0	1	0	0
W. C. Bowman et al. (1982)	2/2	6.6800×10^{-7}	7.96199373640	0	2	0	1
			11.94264828800	0	3	0	2
W. C. Ho et al. (1991)	6/6	0.003	2323.765	1	4	0	5
			2319.607	1	5	0	6
			2289.434	1	12	0	13
			2284.984	1	13	0	14
			2280.492	1	14	0	15
			2262.172	1	18	0	19
G. Hilpert et al. (1994)	2/2	0.005	2378.0890	1	9	0	8
			2385.2328	1	11	0	10
J. Cernicharo et al. (2014)	5/5	2.7722×10^{-6}	7.96199463152	0	2	0	1
			19.90261648	0	5	0	4
			23.88164452	0	6	0	5
			27.85985783	0	7	0	6
			31.83712011	0	8	0	7
O. Asvany et al. (2021)	3/3	2.338×10^{-7}	3.98108879279	0	1	0	0
			7.96199590807	0	2	0	1
			11.94266015702	0	3	0	2

ature were collected. Nine sources were identified; six of them performed laboratory spectroscopy (F. Alberti & A. E. Douglas 1975; W. C. Bowman, E. Herbst & F. C. De Lucia 1982; W. C. Ho et al. 1991; G. Hilpert et al. 1994; G. K. Jarvis et al. 1999; O. Asvany et al. 2021), two observed the upper atmosphere of the Earth (D. R. Smith, E. R. Huppi & J. O. Wise 2000; M. López-Puertas et al. 2006), and one reported pure rotational transitions of NO⁺ in both the laboratory and interstellar medium (J. Cernicharo et al. 2014). However, the observations of D. R. Smith et al. (2000) contain only band heads and therefore were not usable as input into MARVEL. Interestingly, the laboratory spectrum of G. K. Jarvis et al. (1999) featured high resolution photoelectron ionization studies of neutral NO giving transitions to vibrationally-resolved states of the NO⁺ ground state ranging from $v = 0$ to $v = 32$. These photoelectron ionization data were not included in the MARVEL inputs nor in the fitting of the PEC due to high uncertainty values, but the information on the higher vibrational states proves useful for comparison with this work. The seven sources used in this work as inputs into MARVEL and fitting are summarized in Tables 1 and 2. Three sources (W. C. Bowman et al. 1982; J. Cernicharo et al. 2014; O. Asvany et al. 2021) contain hyperfine-resolved pure rotational transitions. However, nuclear spin effects were not considered in this work and transitions corresponding to the same pair of upper and lower rotational states (J) state were averaged over the hyperfine quantum number, F ; this was necessary as none of the observed ro-vibrational transitions are hyperfine resolved.

These seven sources covered transitions from vibrational states $v = 0$ to $v = 2$ with a range of rotational states within those

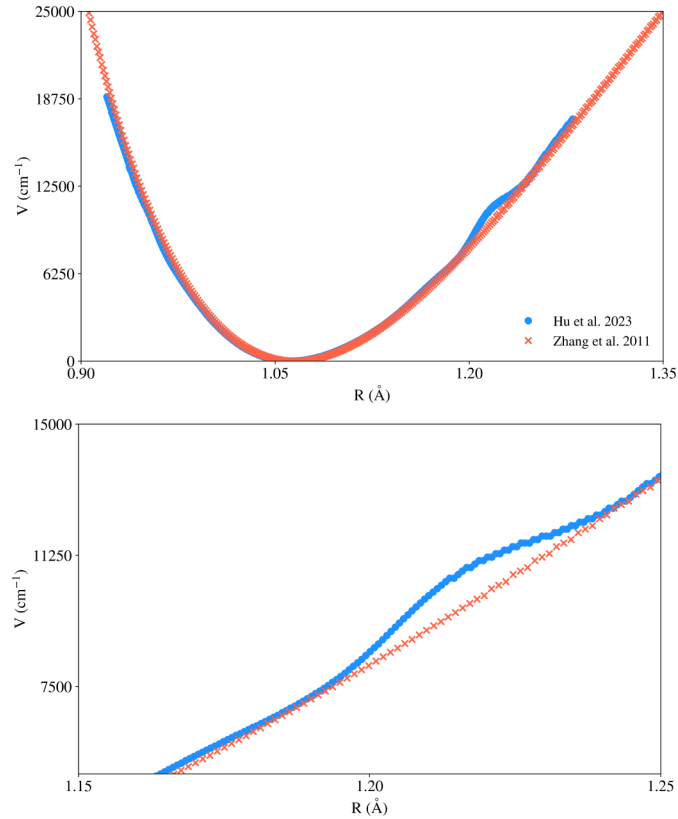
vibrational states. Uncertainties for each transition were initially difficult to locate in the literature sources. Ideally, each observation would have a unique uncertainty assigned to it; however, many of the sources contained only overall uncertainties or did not specify uncertainties at all. For several sources, uncertainties had to be estimated or inferred from other parts of the text. The uncertainty of the W. C. Bowman et al. (1982) pure rotational data was estimated to be 20 kHz based on their corrections for the Doppler effect, which they stated were marginally statistically significant at 20 kHz. The data of M. López-Puertas et al. (2006), see Table 2, were calibrated to the results of a similar paper (M. Kaufmann et al. 2006), and from this the uncertainty was estimated at 0.001 cm⁻¹. G. Hilpert et al. (1994) do not state an error for their observations, so based on the values of the other data in this set, the uncertainty was set at a conservative 0.005 cm⁻¹. The rest of the data sources provided measurement errors that were included as uncertainties.

2.2 Potential energy curve

PECs for the NO⁺ ion ground state were calculated using 11 levels of theory across a total of seven literature sources (H.-J. Werner & P. Rosmus 1982; K. A. Peterson & R. C. Woods 1987; G. Chabaud & P. Rosmus 1990; M. Fehér & P. A. Martin 1993; R. Reddy et al. 2006; J.-P. Zhang et al. 2011; M.-L. Hu et al. 2023). The multireference configuration interaction (MRCI) calculations of J.-P. Zhang et al. (2011) and M.-L. Hu et al. (2023) would appear to be the most accurate on theoretical grounds; PECs for these two sources are compared in Fig. 1. The more recent calculations

Table 2. Summary of Earth observations of NO⁺ from M. López-Puertas et al. (2006). ‘A/V’ is the number of actual lines in the source/number of lines validated by MARVEL.

Source	A/V	Uncertainty (cm ⁻¹)	Transition					Transition				
			Frequency (cm ⁻¹)	v'	J'	v''	J''	Frequency (cm ⁻¹)	v'	J'	v''	J''
M. López-Puertas et al. (2006)	48/48	0.001	2233.650	1	24	0	25	2378.100	1	9	0	8
			2238.500	1	23	0	24	2385.250	1	11	0	10
			2243.300	1	22	0	23	2388.750	1	12	0	11
			2248.075	1	21	0	22	2392.225	1	13	0	12
			2252.800	1	20	0	21	2395.650	1	14	0	13
			2257.500	1	19	0	20	2399.050	1	15	0	14
			2262.175	1	18	0	19	2402.400	1	16	0	15
			2266.800	1	17	0	18	2405.725	1	17	0	16
			2271.400	1	16	0	17	2409.000	1	18	0	17
			2275.975	1	15	0	16	2225.650	2	19	1	20
			2280.500	1	14	0	15	2230.300	2	18	1	19
			2284.975	1	13	0	14	2239.450	2	16	1	17
			2289.450	1	12	0	13	2243.975	2	15	1	16
			2315.400	1	6	0	7	2261.725	2	11	1	12
			2319.600	1	5	0	6	2266.075	2	10	1	11
			2323.775	1	4	0	5	2274.650	2	8	1	9
			2327.900	1	3	0	4	2278.900	2	7	1	8
			2331.975	1	2	0	3	2283.100	2	6	1	7
			2355.725	1	3	0	2	2341.575	2	8	1	7
			2359.550	1	4	0	3	2348.725	2	10	1	9
			2363.325	1	5	0	4	2352.250	2	11	1	10
			2367.075	1	6	0	5	2359.125	2	13	1	12
			2370.800	1	7	0	6	2365.900	2	15	1	14
			2374.450	1	8	0	7	2369.250	2	16	1	15

**Figure 1.** PECs for the X¹Σ⁺ state from DUO potential energy grids based on J.-P. Zhang et al. (2011) (crosses) and M.-L. Hu et al. (2023) (dots).

of M.-L. Hu et al. (2023) contain a $\approx 1500 \text{ cm}^{-1}$ hump at about $1.22 \text{ \AA}$ in their PEC, which was amplified by the DUO interpolation used to provide a potential energy grid; for this reason the smooth PEC of J.-P. Zhang et al. (2011) was chosen as the *ab initio* starting point for the fit with DUO; these calculations also have a higher sampling rate and a larger range of internuclear separations, which improved the robustness and range of DUO interpolation.

2.3 Dipole moment curve

Three different sources used a total of five different methods to calculate the variation of the charge distribution with the NO^+ nuclear geometry and tabulated their results as *ab initio* DMCs (G. Chambaud & P. Rosmus 1990; H.-J. Werner & P. Rosmus 1982; M. Fehér & P. A. Martin 1993). For ions, the dipole moment is origin dependent. The published NO^+ DMCs used differently defined, or undefined, orientation, and origin of their dipoles when presenting their values. To accurately compare the DMCs, we shifted all DMCs to have their origin lying at the NO^+ centre-of-mass and oriented N to O along the axis. A comparison of these DMCs with corrected orientation and origin is given in Fig. 2.

After adjusting the data of G. Chambaud & P. Rosmus (1990) and H.-J. Werner & P. Rosmus (1982), it became clear that two different asymptotes existed depending on the type of calculation performed in the study, meaning that upon dissociation at high internuclear separation the ion dissociates to either $\text{N}^+ + \text{O}$ or $\text{N} + \text{O}^+$. For example, second-order Møller-Plesset (MP2) calculations of the DMC by H.-J. Werner & P. Rosmus (1982) tend asymptotically to $\text{N} + \text{O}^+$. However, the ionization potential of N is lower than that of O, so the dissociation limit should be $\text{N}^+ + \text{O}$ (J. Wu, H. Zeng & C. Guo 2007). Therefore, only DMCs that tend to the $\text{N}^+ + \text{O}$ asymptote were considered. The MRCI and CASSCF DMCs of M. Fehér & P. A. Martin (1993) were originally considered as their calculations are the most recent and span the largest range of internuclear separation. As plotted in Fig. 2, the two data sets are in strong agreement in the $0.5\text{--}1.5 \text{ \AA}$ range – the entire span of the MRCI calculations. However, the CASSCF data of M. Fehér & P. A. Martin (1993) were sampled more densely and spanned a larger range of internuclear separations than the MRCI data. Even though MRCI is a higher level of theory, the CASSCF calculations were chosen because of this increased range and sampling. However, the CASSCF data still did not contain sufficient points for direct input into DUO for calculating intensities of the transitions. Instead of using the raw M. Fehér & P. A. Martin (1993) CASSCF data, a DUO automatic cubic spline interpolation was used between 0.5 and $2.0 \text{ \AA}$, generating 500 points. While this interpolation reproduces the curve well, it was necessary to ensure that the DMC was smooth over the entire data range to prevent noise in the intensity calculations. This DUO spline was compared with longer range interpolations to determine the best method. The PYTHON library SCIPY's interpolation function was used to interpolate more points to give a finer sampling rate. Between the first and final points of the CASSCF data, 1000 points were generated, using linear, quadratic, and cubic interpolation from SCIPY. The cubic spline resulted in the smoothest fit making it the best choice for the input in DUO for calculating the transition intensities. The cubic interpolation is compared to the M. Fehér & P. A. Martin (1993) CASSCF data in Fig. 3.

3 METHODS

The MARVEL (T. Furtenbacher et al. 2007) algorithm inverts transition data to give highly accurate energy levels along with determined uncertainties. DUO (S. N. Yurchenko et al. 2016) is a very general programme for the variational solution of the diatomic nuclear-motion problem. DUO can fit PECs to experimentally determined energy levels, where an extended Morse oscillator (EMO; E. G. Lee et al. 1999) was used to represent the ground state PEC and then refined by minimizing the residual between calculated energy levels and the spectroscopic network of empirically determined levels generated by MARVEL. DUO is then used to compute line intensities for rotational and vibrational transitions. The EXOCROSS programme (S. N. Yurchenko, A. F. Al-Refaie & J. Tennyson 2018) was used to generate transition intensities across a range of temperatures as seen in the cross-section plots in Section 4.3.

3.1 MARVEL energy levels

Using an input of two quantum numbers (v and J), MARVEL2.1 was executed using a numerical matrix inversion algorithm to invert experimental transition frequencies into state energies. Hyperfine transitions were averaged into pure rotational transitions by averaging transition energies with the same upper and lower J values, but different F values. This facilitated merging with other ro-vibrational transition data, which contained only J and v quantum numbers, so that a spectroscopic network between all sources could be established. With a relatively small data set compared to most MARVEL studies, we were able to manually adjust uncertainties outside the programme where necessary.

After data cleaning and adjustment of uncertainties to produce self-consistency, MARVEL produced a spectroscopic network that consisted of nine different components, containing a total of 67 transitions. Each component is a web with associated nodes representing states that are connected by transitions (edges). In an ideal case, all 67 transitions would form a single network. However, because not every state was interconnected by the observed transitions, the network became fragmented into these nine components.

The first component contained the most states. It consisted of 23 states from $v=0$ to $v=2$ levels and ranging from $J=0$ to $J=11$ rotational levels within those vibrational states, and only contained 44 of the 67 transitions input. However, the second and third components also contained several states of use in this analysis, and included the majority of the remaining transitions. We made use of spectroscopic constants from M. López-Puertas et al. (2006) to connect the network components in MARVEL. The energies of the states with $J=10, 11, 12$ and $v=0$ were calculated using the equation

$$E_J^{v=0} = J(J+1)B_0 - (J(J+1)^2)D_0, \quad (1)$$

where $B_0 = 1.98794659 \text{ cm}^{-1}$ and $D_0 = 5.539822 \times 10^{-6} \text{ cm}^{-1}$ given by M. López-Puertas et al. (2006). From the states, we calculated transition frequencies of the $J=12$ to $J=10$ and $J=11$ to $J=10$ transitions. The addition of these transitions to our MARVEL input connected the three network components. The MARVEL input transitions file and output energy file are given in the supplementary information.

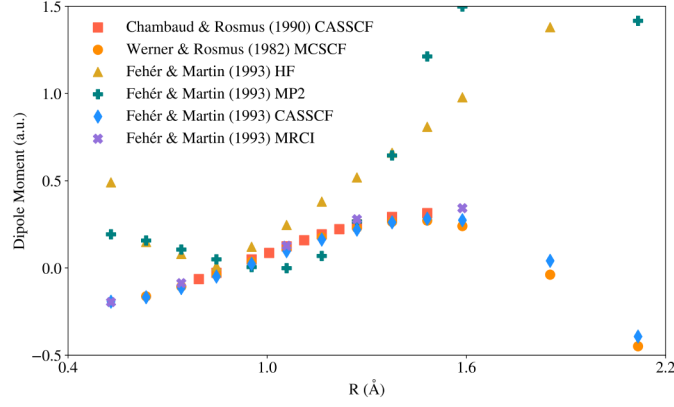


Figure 2. Comparison of DMCs, in au, from H.-J. Werner & P. Rosmus (1982), G. Chambaud & P. Rosmus (1990), and M. Fehér & P. A. Martin (1993).

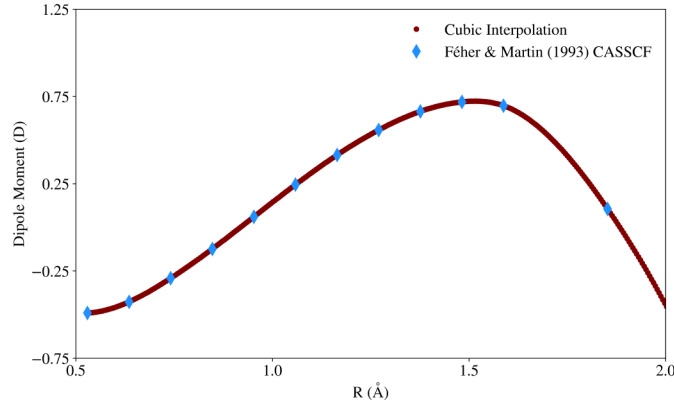


Figure 3. Comparison of dipole moments, in Debye as input into DUO, for the $X^1\Sigma^+$ state. Comparison of CASSCF calculations from M. Fehér & P. A. Martin (1993) and cubic interpolation using SCIPY interpolation.

Table 3. EMO fitting parameters.

Parameter	Value ($\text{\AA}^{-1}$)
a_0	2.692948
a_1	0.0137
a_2	-0.0118

3.2 DUO fitting

DUO was employed to fit a PEC simultaneously to the *ab initio* points and MARVEL spectroscopic network. The EMO fitting function of DUO makes an approximation of an anharmonic PEC by the equation:

$$V(r) = T_e + (A_e - T_e) \left(1 - e^{-\beta_{\text{EMO}}(r)(r-r_e)}\right)^2, \quad (2)$$

where $V(r)$ is the potential as a function of r , the internuclear separation, and r_e , the equilibrium internuclear separation. T_e is the minimum energy of the potential well. A_e represents the dissociation asymptote at r approaching infinity, given by the dissociation energy in this case (S. N. Yurchenko et al. 2016). The exponent is then given by the following expansion

$$\beta_{\text{EMO}} = \sum_{i=0}^N a_i y_p^{eq}(r)^i \quad (3)$$

with $N + 1$ adjustable fitting parameters, a_i . Note that if $N = 0$, β_{EMO} is a constant and equation (2) becomes the simple Morse expression. The Šurkus variable (A. A. Šurkus, R. J. Rakauskas & A. B. Bolotin 1984) is given by

$$y_p^{eq}(r) = \frac{r^p - r_e^p}{r^p + r_e^p}. \quad (4)$$

The variable $r_e = 1.063 \text{ \AA}$ (given by J.-P. Zhang et al. 2011 and then fit) represents the equilibrium internuclear separation (S. N. Yurchenko et al. 2016). The EMO approximation was fit to the MARVEL output data as well as the *ab initio* PEC, which is the grid interpolated output of the MRCI calculations of J.-P. Zhang et al. (2011). The parameter A_e was fixed to 86244.82 cm^{-1} based on R. Reddy et al. (2006). Parameter p , the exponent term, was fixed for both left and right sides of equilibrium at 4 as this provided the best fit. The EMO was best fit by two terms on each side of equilibrium, listed in Table 3. The same values of each term are used to fit both sides of equilibrium.

4 RESULTS

4.1 Line list and file structure

The NOPE (N O Plus, and the lead author's first initial) line list was generated using the DUO programme, computing rotational states up to $J = 100$ and vibrational states up to $v = 41$ from the fitted PEC described in Section 3.2. This yielded a total of 3881

Table 4. Extract from the states file for the NOPE line list.

i	$\tilde{E}$	g_i	J	unc	τ	p	e/f	v	calc	Label
736	62710.34066	63	10	6.35	0.00608	+	e	35	62710.34066	Ca
737	63905.67210	63	10	6.5	0.00597	+	e	36	63905.67210	Ca
738	65068.20233	63	10	6.65	0.00588	+	e	37	65068.20233	Ca
739	66197.93816	63	10	6.8	0.00579	+	e	38	66197.93816	Ca
740	67294.95624	63	10	6.95	0.00572	+	e	39	67294.95624	Ca
741	68359.89144	63	10	7.1	0.00566	+	e	40	68359.89144	Ca
742	69396.40140	63	10	7.25	0.00554	+	e	41	69396.40140	Ca
771	262.3124241	69	11	0.0484636	1180	–	e	0	262.338074	EH
772	2603.978273	69	11	0.0302413	0.0929	–	e	1	2603.937846	Ma
773	4912.908325	69	11	0.0504636	0.0478	–	e	2	4912.903532	Ma
774	7189.216106	69	11	1.77	0.0328	–	e	3	7189.216106	Ca
775	9432.858016	69	11	1.92	0.0253	–	e	4	9432.858016	Ca
776	11643.81470	69	11	2.07	0.0208	–	e	5	11643.81470	Ca
777	13822.07298	69	11	2.22	0.0179	–	e	6	13822.07298	Ca
778	15967.62113	69	11	2.37	0.0158	–	e	7	15967.62113	Ca

Notes: i : State counting number.

$\tilde{E}$: State energy (in cm^{-1}).

g_i : Total statistical weight, equal to $g_{\text{ns}}(2J + 1)$.

J : Total angular momentum quantum number.

Unc: Uncertainty (in cm^{-1}). Determined for calculated states by $\text{Unc} = a v + b J(J + 1)$ where $a = 0.15 \text{ cm}^{-1}$ and $b = 0.01 \text{ cm}^{-1}$.

τ : Lifetime (in s).

p : Total parity.

e/f : Rotationless parity.

v : Vibrational Quantum Number.

Calc: Original DUO calculated state energy (in cm^{-1}).

Label: ‘Ma’ for MARVEL, ‘Ca’ for calculated, ‘EH’ for Effective Hamiltonian (L. K. McKemmish et al. 2024).

Table 5. Extract from the transitions file for the NOPE line list.

f	i	$A_{fi} (\text{s}^{-1})$	$\tilde{\nu}_{fi} (\text{cm}^{-1})$
89	19	7.5432E–07	3.278429
88	18	7.5214E–07	3.318775
87	17	7.4760E–07	3.358917
86	16	7.4077E–07	3.398861
85	15	7.3174E–07	3.438608
84	14	7.2058E–07	3.478165
83	13	7.0742E–07	3.517533
82	12	6.9239E–07	3.556717
81	11	6.7563E–07	3.595719
80	10	6.5728E–07	3.634543
79	9	6.3750E–07	3.673191
78	8	6.1643E–07	3.711666

Notes: f : Upper state counting number.

i : Lower state counting number.

A_{fi} : Einstein- A coefficient (in s^{-1}).

$\tilde{\nu}_{fi}$: Transition wavenumber (in cm^{-1}).

states and 54 434 transitions. The resulting line list is stored in ExoMol format (J. Tennyson, C. Hill & S. N. Yurchenko 2013; J. Tennyson et al. 2024) as a states file and a transitions file, excerpts of which are provided in Tables 4 and 5, respectively.

4.2 Partition functions

A partition function for NO^+ is provided by the HITRAN data base up to 5000 K (R. R. Gamache et al. 2025) and the partition function for NO^+ was calculated using the ExoCROSS program (S. N. Yurchenko et al. 2018) in steps of 1 K up to 5000 K. The ExoMol convention, in accordance with HITRAN (R. R. Gamache et al. 2017), is to provide partition functions that include full atomic nuclear spin degeneracy, g_{ns} , which in this case has a value

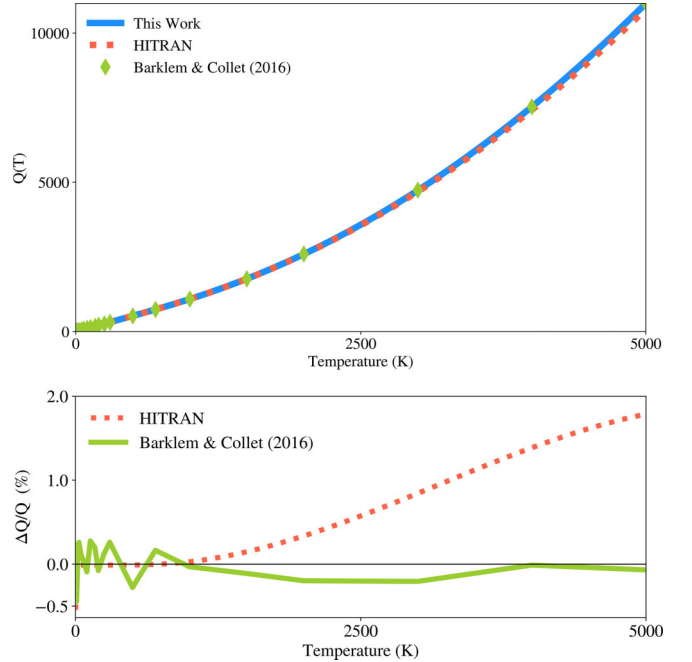


Figure 4. NO^+ partition function as calculated from the NOPE line list using ExoCROSS compared with that of HITRAN (R. R. Gamache et al. 2025) (dashed lines) and P. S. Barklem & R. Collet (2016) (diamonds, solid line). Percentage differences are calculated as this work minus R. R. Gamache et al. (2025) or P. S. Barklem & R. Collet (2016).

of 3. The P. S. Barklem & R. Collet (2016) dataset does not initially include the degeneracy, so its values were multiplied by a factor of 3 for comparison. The partitions functions for the NOPE line list, the HITRAN line list and the P. S. Barklem & R. Collet (2016)

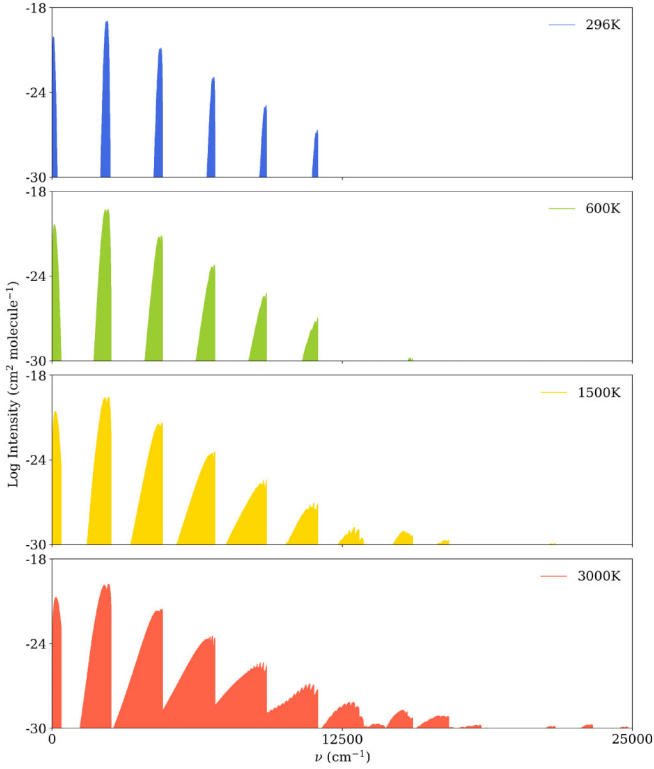


Figure 5. Intensities calculated using the NOPE line list and EXOCROSS at $T = 296, 600, 1500, 3000$ K.

data are compared in Table Table 6. Fig. 4 displays the functions and their relative percentage differences from 0 to 5000 K. At high temperature the HITRAN partition function is lower than the other two, potentially an underestimate which appears to be a common feature (R. Wang et al. 2023). The NOPE line list is more complete than the HITRAN line list, as well. The agreement between our partition function and that of P. S. Barklem & R. Collet (2016) is good.

Table 6. Comparison of the transition information between this work and HITRAN (I. E. Gordon et al. 2026).

Line list	Maximum ν	Maximum J	Number of states	Number of transitions
NOPE	41	100	3881	54434
HITRAN	6	101	713	1270

Table 7. Partition function comparison.

$T(K)$	$Q(T)$		
	This work	HITRAN	P. S. Barklem & R. Collet (2016)
296	311.6222	311.65635	N/A
1000	1089.6578	1089.3474	1090.0
1750	2162.0041	2156.9488	N/A
2000	2594.8551	2586.1575	2600.0
3000	4730.2599	4690.6855	4740.0
4000	7529.1339	7426.1423	7530.0
5000	10992.4257	10799.394	11000.0

4.3 Spectra

Intensities for this line list calculated with EXOCROSS at increasing temperatures are presented in Fig. 5 as stick spectra (no line broadening). In semilog space, Fig. 5 shows a linear decrease in the rovibrational spectrum with transition frequency. The exception occurs at high temperatures (>1500 K), where the high-frequency overtone bands begin to flatten in intensity. This flattening occurs because the inherently weak overtone intensities drop into the numerical noise floor of the grid-based dipole data. While this noise can be overcome by fitting the dipole to an analytical form (E. S. Medvedev et al. 2015, 2016; E. S. Medvedev & V. G. Ushakov 2022), the effect remains small in our model and is negligible at lower temperatures where these states are not thermally populated.

5 DISCUSSION AND CONCLUSIONS

To assess the quality of the calculated line list, comparisons with previously determined spectra are made. A comparison of the transition information between this work and HITRAN is made in Table Table 7. Strong agreement in line positions and intensities between the existing HITRAN line list and this work, where the two overlap, is visible in Fig. 7. The HITRAN NO⁺ line list uses the H.-J. Werner & P. Rosmus (1982) DMC, which accounts for the minor differences in the intensities of the two sources. The standard deviation between transition energies of the two sources is 0.093 cm^{-1} implying close agreement for line locations. Further statistics are presented in Table 8.

This work also agrees with laboratory and Earth atmosphere observational sources. The G. K. Jarvis et al. (1999) $\nu = 0$ to $\nu = 32$ state energies (with $J = 0$ assumed) observed in the laboratory via photoelectron ionization are compared with the NOPE line list levels up to $\nu = 41$ in Fig. 8. Agreement is strong between the Earth atmosphere observations in M. López-Puertas et al. (2006) and this work as well. The mean difference between the line positions of the two was 0.066 cm^{-1} . The full comparison is presented in Table 9.

To conclude, the NOPE line list for the rotational and rovibrational transitions of the ground electronic state of $^{14}\text{N}^{16}\text{O}^+$ has been constructed using a refined spectroscopic model. As there

Table 8. Mean residuals and standard deviations between this work and HITRAN.

	Mean of residuals	Standard deviation
E (cm ⁻¹)	0.0797	0.0930
Intensity (cm ² molecule ⁻¹)	-3.661E-22	1.569E-21
Einstein A Coefficient (s ⁻¹)	0.079	0.231

Table 9. Comparison of this work with the Earth spectrum observed in M. López-Puertas et al. (2006).

ν	Upper state		Lower state		$E(\text{cm}^{-1})$	This work	Difference
	J	ν	J	M. López-Puertas et al. (2006)			
1	24	0	25	2233.65	2233.807778	0.157778	
1	23	0	24	2238.5	2238.640015	0.140015	
1	22	0	23	2243.3	2243.438041	0.138041	
1	21	0	22	2248.075	2248.201734	0.126734	
1	20	0	21	2252.8	2252.930972	0.130972	
1	19	0	20	2257.5	2257.625632	0.125632	
1	18	0	19	2262.175	2262.285589	0.110589	
1	17	0	18	2266.8	2266.910721	0.110721	
1	16	0	17	2271.4	2271.500901	0.100901	
1	15	0	16	2275.975	2276.056004	0.081004	
1	14	0	15	2280.5	2280.575903	0.075903	
1	13	0	14	2284.975	2285.060473	0.085473	
1	12	0	13	2289.45	2289.509585	0.059585	
1	6	0	7	2315.4	2315.452431	0.052431	
1	5	0	6	2319.6	2319.649719	0.049719	
1	4	0	5	2323.775	2323.810509	0.035509	
1	3	0	4	2327.9	2327.934666	0.034666	
1	2	0	3	2331.975	2332.022058	0.047058	
1	3	0	2	2355.725	2355.766793	0.041793	
1	4	0	3	2359.55	2359.593043	0.043043	
1	5	0	4	2363.325	2363.38144	0.05644	
1	6	0	5	2367.075	2367.131845	0.056845	
1	7	0	6	2370.8	2370.844119	0.044119	
1	8	0	7	2374.45	2374.518122	0.068122	
1	9	0	8	2378.1	2378.153713	0.053713	
1	11	0	10	2385.25	2385.30910	0.05910	
1	12	0	11	2388.75	2388.828612	0.078612	
1	13	0	12	2392.225	2392.309146	0.084146	
1	14	0	13	2395.65	2395.750559	0.100559	
1	15	0	14	2399.05	2399.152708	0.102708	
1	16	0	15	2402.4	2402.515448	0.115448	
1	17	0	16	2405.725	2405.838634	0.113634	
1	18	0	17	2409.0	2409.122122	0.122122	
2	19	1	20	2225.65	2225.717474	0.067474	
2	18	1	19	2230.3	2230.343231	0.043231	
2	16	1	17	2239.45	2239.489659	0.039659	
2	15	1	16	2243.975	2244.01008	0.03508	
2	11	1	12	2261.725	2261.736846	0.011846	
2	10	1	11	2266.075	2266.079168	0.004168	
2	8	1	9	2274.65	2274.655661	0.005661	
2	7	1	8	2278.9	2278.889572	−0.010428	
2	6	1	7	2283.1	2283.087084	−0.012916	
2	8	1	7	2341.575	2341.590599	0.015599	
2	10	1	9	2348.725	2348.745377	0.020377	
2	11	1	10	2352.25	2352.264535	0.014535	
2	13	1	12	2359.125	2359.185676	0.060676	
2	15	1	14	2365.9	2365.949625	0.049625	
2	16	1	15	2369.25	2369.272290	0.022290	

Note. Difference: calculated as this work minus M. López-Puertas et al. (2006).

are currently no high temperature line lists available for NO⁺, the goal of this study was to produce such a line list. The NOPE line list is available from www.exomol.com. The results of this study

should assist future studies aiming to characterize planetary and exoplanetary atmospheres, particularly ionospheres, from spectroscopic information.

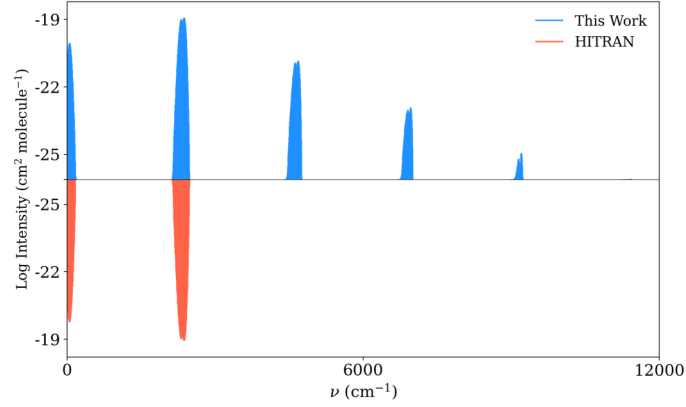


Figure 6. NOPE line list intensities calculated with EXOCROSS compared with HITRAN line positions and intensities at 296 K. HITRAN is presented below the x-axis and this work above. Minimum intensity threshold of 10^{-30} cm² per molecule.

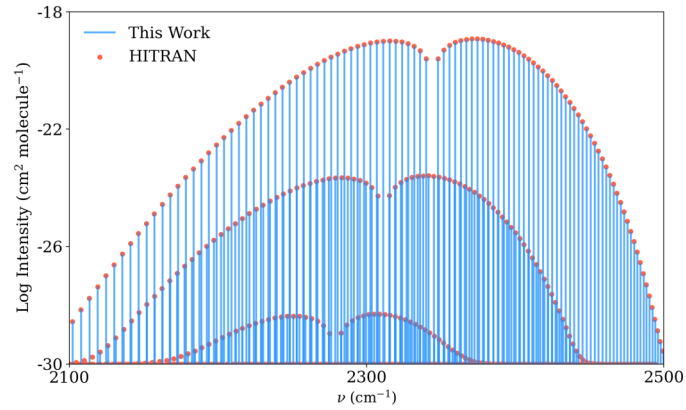


Figure 7. Comparison of NOPE line list intensities from EXOCROSS with HITRAN intensities at 296 K at the 2300 cm⁻¹ peak. HITRAN is shown as dots and this work in vertical lines. Minimum intensity threshold of 10^{-30} cm² per molecule.

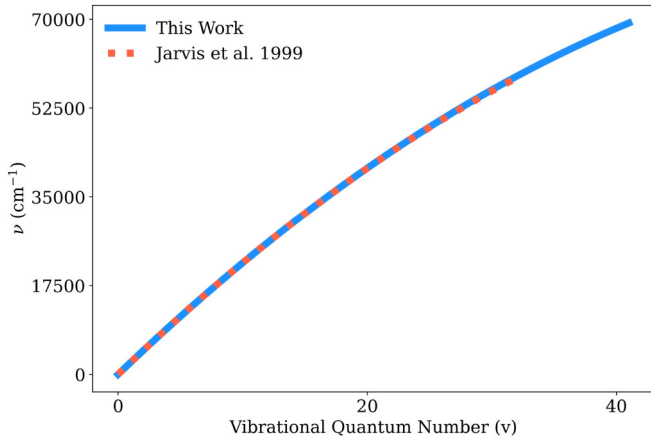


Figure 8. Comparison of the $J = 0, v = 0$ to $v = 41$ states for this work (solid line) and the original G. K. Jarvis et al. (1999) data (dashed line). The Jarvis states were observed up to a maximum of $v = 32$.

CONFLICT OF INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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DATA AVAILABILITY

The states, transition and partition function files for the ¹⁴N¹⁶O⁺ line list can be downloaded from www.exomol.com. All other supporting data are provided in the paper or supporting materials.

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SUPPLEMENTARY MATERIAL

Supplementary data are available at *MNRAS* online.

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