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Einstein A-coefficients for rotational transitions in the HN_2O^+

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Abstract. Einstein A-values for the electric dipole transitions between the rotational levels up to $540\,\mathrm{cm}^{-1}$ and $J = 11$ in the ground vibrational state of the protonated N_2O (i.e., HN_2O^+) are calculated. The coefficients are used to compute the mean radiative lifetimes of the levels. These A-values can be used for analysing the spectra from astronomical objects, if observed.

Keywords. Einstein A-coefficients; rotational transitions; asymmetric top molecule; HN_2O^+-molecule.

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1. Introduction

A number of molecules have been observed in the astronomical objects. Some of them have been even found in the vibrationally excited states. For analysing the spectra from astronomical objects, the Einstein A-values are one of the important parameters [1, 2 and references cited therein]. Bogey *et al* [3] made predictions of some rotational transitions of HN_2O^+ (protonated nitrous oxide) that may be of astrophysical interest. They used magnetically confined negative glow discharge to investigate the millimeter wave spectrum of HN_2O^+ in the 132–290 GHz. They also derived the rotational and distortional molecular constants. Since the molecule may be of astrophysical interest, the analysis of the observations would require the knowledge of transition probabilities (i.e., the Einstein A-values). Therefore, in the present communication we have calculated the Einstein A-coefficients for the electric dipole transitions between the rotational levels up to $540\,\mathrm{cm}^{-1}$ and $J = 11$.

2. Einstein A-coefficients for HN_2O^+

The HN_2O^+ is a a-type asymmetric top molecule with dipole moment $\mu = 2{\cdot}4\,\mathrm{D}$. Details of the calculations of Einstein A-values for a-type asymmetric top molecules are the same as published in Chandra *et al* [1] and Jaruschewski *et al* [4]. The rotational wave functions for the asymmetric top molecule can be described by linear combinations of symmetric top wave functions:

$$\psi_{J\tau M}(\alpha,\beta,\gamma) = \left(\frac{2J+1}{8\pi^2}\right)^{1/2} \sum_{K=-J}^{J} g^J_{\tau K} D^J_{MK}(\alpha,\beta,\gamma) \tag{1}$$

where α, β, γ are the Eulerian angles specifying the orientation of the molecule, J the rotational quantum number, $g^J_{\tau K}$ the expansion coefficients, D^J_{MK} the Wigner D-functions, and the pseudo quantum number τ is defined by

$$\tau = K_{-1} - K_{+1}. \tag{2}$$

The rotational transitions are governed by the selection rules

$$J: \Delta J = 0, \quad \pm 1$$

$$K_{-1}, \quad K_{+1}: \quad \text{odd, even} \leftrightarrow \text{odd, odd}$$

$$\text{even, odd} \leftrightarrow \text{even, even.}$$

In the representation in which the axis of quantization is along the a-axis of inertia, the expression for the line strength is given by

$$S(J'_{\tau'} \to J_\tau) = \mu^2(2J+1)\left[\sum_{K=-J}^{J} g^J_{\tau K} g^{J'}_{\tau' K} C^{J'K}_{JK10}\right]^2 \tag{3}$$

where the C's are Clebsch–Gordan coefficients. The transition probabilities follow directly from the line strength

$$A(J'_{\tau'} \to J_\tau) = \frac{64\pi^4 \nu^3 S(J'_{\tau'} \to J_\tau)}{3hc^3(2J'+1)} \tag{4}$$

where the frequency ν corresponds to the energy difference of the two levels.

3. Molecular constants

The molecular constants for the ground vibrational state of the protonated N_2O are reported by Bogey *et al* [3], and are given in table 1.

4. Results and discussion

The calculated values of the Einstein A-coefficients for the trnasitions $J'\tau' \to J\tau$ are given in tables 2 and 3. Here the primed parameters correspond to the upper level

Table 1. Molecular constants for protonated N_2O.

A	623923·(1420)[a]	MHz
B	11301·5587(19)	MHz
C	11084·2784(19)	MHz
D_J	5·3371(30)	kHz
D_{JK}	726·54(83)	kHz
D_K	242·8	kHz
d_1	− 0·0910(34)	kHz
d_2	− 0·0240(33)	kHz
H_{KJ}	0·35(11)	kHz
L_{KJ}	0·0891(46)	kHz

[a]Numbers in parentheses represent one standard deviation in unit of the last quoted digit.

Table 2. Einstein A-coefficients for ortho-HN_2O^+.

J'	τ'	J	τ	$A(s^{-1})$	J'	τ'	J	τ	$A(s^{-1})$	J'	τ'	J	τ	$A(s^{-1})$
1	1	1	0	3·4387D − 13	2	−1	1	0	1·7785D − 06	2	0	1	1	1·8311D − 06
2	0	2	−1	3·0949D − 12	3	−2	2	−1	7·6221D − 06	3	−1	2	0	7·8473D − 06
3	−1	3	−2	1·2380D − 11	4	−3	3	−2	1·9760D − 05	4	−2	3	−1	2·0344D − 05
4	−2	4	−3	3·4390D − 11	5	−4	4	−3	4·0418D − 05	5	−3	4	−2	4·1612D − 05
5	−3	5	−4	7·7381D − 11	6	−5	5	−4	7·1817D − 05	6	−4	5	−3	7·3940D − 05
6	−4	6	−5	1·5168D − 10	7	−6	6	−5	1·1618D − 04	7	−5	6	−4	1·1961D − 04
7	−5	7	−6	2·6966D − 10	8	−7	7	−6	1·7572D − 04	8	−6	7	−5	1·8092D − 04
8	−6	8	−7	4·4581D − 10	9	−8	8	−7	2·4031D − 04	9	−7	8	−6	3·6756D − 05
9	−7	9	−8	3·2655D − 13	10	−9	9	−8	2·8143D − 04	10	−8	9	−7	1·1192D − 04
10	−8	10	−9	8·4718D − 10	11	−10	10	−9	3·9649D − 11	11	−9	11	−10	1·8139D − 07
3	2	2	−1	2·3085D − 08	3	2	3	−1	1·9395D − 08	3	2	4	−3	4·7174D − 09
3	3	2	0	2·3088D − 08	3	3	3	−2	1·9390D − 08	3	3	4	−2	4·7194D − 09
4	1	3	−2	4·7767D − 08	4	1	4	−2	4·8879D − 08	4	1	5	−4	1·3506D − 08
4	1	3	2	9·3429D − 06	4	2	3	−1	4·7780D − 08	4	2	4	−3	4·8858D − 08
4	2	5	−3	1·3514D − 08	4	2	3	3	9·3429D − 06	5	0	4	−3	7·6042D − 08
5	0	5	−3	8·6903D − 08	5	0	6	−5	2·5939D − 08	5	0	4	1	2·7300D − 05
5	1	4	−2	7·6078D − 08	5	1	5	−4	8·6845D − 08	5	1	6	−4	2·5961D − 08
5	1	4	2	2·7300D − 05	6	−1	5	−4	1·0866D − 07	6	−1	6	−4	1·3303D − 07
6	−1	7	−6	4·1729D − 08	6	−1	5	0	5·6131D − 05	6	0	5	−3	1·0874D − 07
6	0	6	−5	1·3290D − 07	6	0	7	−5	4·1776D − 08	6	0	5	1	5·6131D − 05
7	−2	6	−5	1·4605D − 07	7	−2	7	−5	1·8709D − 07	7	−2	8	−7	6·0652D − 08
7	−2	6	−1	9·8092D − 05	7	−1	6	−4	1·4620D − 07	7	−1	7	−6	1·8686D − 07
7	−1	8	−6	6·0738D − 08	7	−1	6	0	9·8092D − 05	8	−3	7	−6	1·8849D − 07
8	−3	8	−6	2·4902D − 07	8	−3	9	−8	7·9078D − 08	8	−3	7	−2	1·5543D − 04
8	−2	7	−5	1·8874D − 07	8	−2	8	−7	2·4862D − 07	8	−2	9	−7	1·3600D − 08
8	−2	7	−1	1·5543D − 04	9	−3	8	−6	2·3664D − 07	9	−3	9	−8	1·9183D − 06
9	−3	10	−8	4·2039D − 08	9	−3	8	−2	2·3041D − 04	9	−4	8	−7	2·3622D − 07
9	−4	9	−7	4·6135D − 07	9	−4	10	−9	4·9071D − 08	9	−4	8	−3	2·3041D − 04
10	−5	9	−8	4·3963D − 07	10	−5	10	−8	1·6578D − 06	10	−5	9	−4	3·2526D − 04

10	−4	9	−7	3·2434D−07	10	−4	10	−9	1·0573D−06	10	−4	9	−3	3·2526D−04
11	−5	10	−8	2·9546D−11	11	−5	11	−10	7·2724	11	−5	10	−4	2·0638D−07
11	−6	10	−9	1·5443D−08	11	−6	11	−9	6·6712	11	−6	10	−5	2·9232D−05
11	−6	11	−5	3·7478D−11	5	5	4	2	1·0506D−07	5	5	5	0	4·6539D−08
5	5	6	0	6·7657D−09	5	4	4	1	1·0506D−07	5	4	5	1	4·6539D−08
5	4	6	−1	6·7657D−09	6	3	5	0	2·0509D−07	6	3	6	0	1·2188D−07
6	3	7	−2	2·1440D−08	6	3	5	4	2·2806D−05	6	4	5	1	2·0509D−07
6	4	6	−1	1·2188D−07	6	4	7	−1	2·1440D−08	6	4	5	5	2·2806D−05
7	3	7	−6	1·4935D−13	7	3	6	0	3·0675D−07	7	3	7	−2	2·1938D−07
7	3	8	−2	4·4033D−08	7	3	6	4	5·8695D−05	7	2	6	−1	3·0675D−07
7	2	7	−1	2·1938D−07	7	2	8	−3	4·4033D−08	7	2	6	3	5·8695D−05
8	2	8	−7	1·0005D−13	8	2	7	−1	4·1326D−07	8	2	8	−3	3·3607D−07
8	2	9	−3	7·4303D−08	8	2	7	3	1·0992D−04	8	1	8	−6	3·3696D−13
8	1	7	−2	4·1326D−07	8	1	8	−2	3·3607D−07	8	1	9	−4	7·4303D−08
8	1	7	2	1·0992D−04										

Table 3. Einstein A-coefficients for para-HN_2O^+.

J'	τ'	J	τ	$A(s^{-1})$	J'	τ'	J	τ	$A(s^{-1})$	J'	τ'	J	τ	$A(s^{-1})$
1	−1	0	˙0	2·5070D−07	2	−2	1	−1	2·4067D−06	3	−3	2	−2	8·7025D−06
4	−4	3	−3	2·1392D−05	5	−5	4	−4	4·2728D−05	6	−6	5	−5	7·4967D−05
7	−7	6	−6	1·2036D−04	8	−8	7	−7	1·4894D−04	9	−9	8	−8	1·8619D−05
10	−10	9	−9	2·2759D−12	11	−11	10	−10	8·1222D−05	2	1	2	−2	1·5515D−08
2	2	1	−1	9·8283D−09	2	2	3	−3	5·7096D−09	3	0	3	−3	3·8786D−08
3	0	2	1	4·8310D−06	3	1	2	−2	2·4036D−08	3	1	4	−4	1·4866D−08
3	1	2	2	4·8311D−06	4	−1	4	−4	6·9813D−08	4	−1	3	0	1·6032D−05
4	0	3	−3	4·3193D−08	4	0	5	−5	2·6968D−08	4	0	3	1	1·6032D−05
5	−2	5	−5	1·0859D−07	5	−2	4	−1	3·5865D−05	5	−1	4	−4	6·7724D−08

5	−1	6	−6	4·1682D−08	5	−1	4	0	3·5866D−05	6	−3	6	−6	1·5513D−07
6	−3	5	−2	6·6588D−05	6	−2	5	−5	9·8029D−08	6	−2	7	−7	5·8723D−08
6	−2	5	−1	6·6591D−05	7	−4	7	−7	2·0941D−07	7	−4	6	−3	1·1046D−04
7	−3	6	−6	1·3451D−07	7	−3	8	−8	6·5558D−08	7	−3	6	−2	1·1046D−04
8	−5	8	−8	2·0430D−07	8	−5	7	−4	1·6972D−04	8	−4	7	−7	1·7756D−07
8	−4	9	−9	7·3886D−08	8	−4	7	−3	1·6973D−04	9	−6	9	−9	8·6872D−08
9	−6	8	−5	2·4663D−04	9	−5	8	−8	1·0657D−08	9	−5	8	−4	2·4665D−04
10	−6	9	−9	7·7178D−10	10	−6	11	−11	6·5412D−02	10	−6	9	−5	5·3744D−07
10	−7	10	−10	7·9899D−01	10	−7	9	−6	3·2623D−05	10	−7	10	−6	1·6218D−10
11	−7	10	−10	1·0893D−01	11	−7	10	−6	8·0527D−05	11	−8	11	−11	3·1520D−01
11	−8	10	−7	1·3026D−04	11	−8	11	−7	1·3706D−08	4	3	3	0	5·6305D−08
4	3	4	0	3·2579D−08	4	3	5	−2	5·9264D−09	4	4	3	1	5·6305D−08
4	4	4	−1	3·2579D−08	4	4	5	−1	5·9264D−09	5	2	4	−1	1·1156D−07
5	2	5	−1	8·3771D−08	5	2	6	−3	1·8015D−08	5	2	4	3	1·5337D−05
5	3	4	0	1·1156D−07	5	3	5	−2	8·3771D−08	5	3	6	−2	1·8015D−08
5	3	4	4	1·5337D−05	6	1	6	−6	1·4099D−13	6	1	5	−2	1·7008D−07
6	1	6	−2	1·4958D−07	6	1	7	−4	3·5955D−08	6	1	5	2	4·1526D−05
6	2	5	−1	1·7008D−07	6	2	6	−3	1·4958D−07.	6	2	7	−3	3·5955D−08
6	2	5	3	4·1526D−05	7	0	7	−7	4·0091D−13	7	0	6	−3	2·3370D−07
7	0	7	−3	2·2852D−07	7	0	8	−5	5·9425D−08	7	0	6	1	8·0823D−05
7	1	6	−6	2·3051D−13	7	1	8	−8	1·2139D−13	7	1	6	−2	2·3370D−07
7	1	7	−4	2·2852D−07	7	1	8	−4	5·9425D−08	7	1	6	2	8·0823D−05
8	−1	8	−8	7·1563D−13	8	−1	7	−4	3·0340D−07	8	−1	8	−4	3·1991D−07
8	−1	9	−6	8·8143D−08	8	−1	7	0	1·3548D−04	8	0	7	−7	5·2628D−13
8	0	9	−9	3·6451D−13	8	0	7	−3	3·0340D−07	8	0	8	−5	3·1991D−07
8	0	9	−5	8·8141D−08	8	0	7	1	1·3548D−04	9	−2	9	−9	1·1368D−12
9	−2	8	−5	3·7978D−07	9	−2	9	−5	4·2341D−07	9	−2	10	−7	1·3698D−08
9	−2	8	−1	2·0774D−04	9	−1	8	−8	1·4518D−12	9	−1	8	−4	3·7977D−07
9	−1	9	−6	4·2342D−07	9	−1	10	−6	2·3054D−10	9	−1	8	0	2·0774D−04
10	−2	11	−11	1·2646D−05	10	−2	9	−5	4·6324D−07	10	−2	10	−7	4·7673D−05
10	−2	11	−7	5·2613D−06	10	−2	9	−1	2·9986D−04	10	−3	10	−10	2·1023D−05
10	−3	9	−6	4·6325D−07	10	−3	10	−6	8·6727D−06	10	−3	11	−8	7·3368D−08
10	−3	9	−2	2·9986D−04	11	−3	10	−10	7·3914D−05	11	−3	10	−6	3·1559D−05
11	−3	11	−8	1·2337D−04	11	−3	10	−2	4·1406D−04	11	−4	11	−11	3·2729D−06
11	−4	10	−7	4·0272D−07	11	−4	11	−7	1·4460D−06	11	−4	10	−3	4·1407D−04

Table 4. Energies and radiative lifetimes for ortho- and para-levels of HN_2O^+.

J'	τ'	E(cm^{-1})	T(s)	J'	τ'	E(cm^{-1})	T(s)
1	0	21·1815	—	0	0	0·0	—
1	1	21·1888	2·908D + 12	1	−1	0·7467	3·989D + 06
2	−1	22·6676	5·623D + 05	2	−2	2·2401	4·155D + 05
2	0	22·6893	5·461D + 05	3	−3	4·4802	1·149D + 05
3	−2	24·8967	1·312D + 05	4	−4	7·4670	4·675D + 04
3	−1	24·9402	1·274D + 05	5	−5	11·2004	2·340D + 04
4	−3	27·8688	5·061D + 04	6	−6	15·6805	1·334D + 04
4	−2	27·9413	4·915D + 04	7	−7	20·9071	8·308D + 03
5	−4	31·5839	2·474D + 04	8	−8	26·8357	6·714D + 03
5	−3	31·6926	2·403D + 04	9	−9	33·3443	5·371D + 04
6	−5	36·0419	1·392D + 04	10	−10	40·5912	4·394D + 11
6	−4	36·1942	1·352D + 04	11	−11	48·7430	1·231D + 04
7	−6	41·2429	8·607D + 03	2	1	83·9933	6·446D + 07
7	−5	41·4459	8·360D + 03	2	2	83·9933	6·436D + 07
8	−7	47·1868	5·691D + 03	3	0	86·2329	2·053D + 05
8	−6	47·4478	5·527D + 03	3	1	86·2329	2·053D + 05
9	−8	53·8575	4·161D + 03	4	−1	89·2189	6·211D + 04
9	−7	53·8789	2·721D + 04	4	0	89·2189	6·210D + 04
10	−9	61·2105	3·553D + 03	5	−2	92·9514	2·780D + 04
10	−8	61·6303	8·935D + 03	5	−1	92·9515	2·780D + 04
11	−10	69·0172	2·522D + 10	6	−3	97·4303	1·498D + 04
11	−9	69·4957	5·513D + 06	6	−2	97·4305	1·498D + 04
3	2	188·4233	2·119D + 07	7	−4	102·6557	9·036D + 03
3	3	188·4233	2·119D + 07	7	−3	102·6560	9·036D + 03
4	1	191·4084	1·058D + 05	8	−5	108·6275	5·885D + 03
4	2	191·4084	1·058D + 05	8	−4	108·6279	5·883D + 03
5	0	195·1397	3·638D + 04	9	−6	115·3456	4·053D + 03
5	1	195·1397	3·638D + 04	9	−5	115·3462	4·054D + 03
6	−1	199·6173	1·773D + 04	10	−6	122·3664	1·529D + 01
6	0	199·6173	1·773D + 04	10	−7	122·4144	1·252
7	−2	204·8410	1·015D + 04	11	−7	130·5217	9·173
7	−1	204·8410	1·015D + 04	11	−8	130·8120	3·171
8	−3	210·8109	6·412D + 03	4	3	334·4732	1·055D + 07
8	−2	210·8109	6·415D + 03	4	4	334·4732	1·055D + 07
9	−3	217·5270	4·299D + 03	5	2	338·2029	6·431D + 04
9	−4	217·5270	4·326D + 03	5	3	338·2029	6·431D + 04
10	−5	224·9891	3·055D + 03	6	1	342·6786	2·388D + 04
10	−4	224·9891	3·061D + 03	6	2	342·6786	2·388D + 04
11	−5	232·8100	1·375D − 01	7	0	347·9001	1·229D + 04
11	−6	232·8390	1·499D − 01	7	1	347·9001	1·229D + 04
5	5	522·1409	6·315D + 06	8	−1	353·8675	7·343D + 03
5	4	522·1409	6·315D + 06	8	0	353·8675	7·343D + 03
6	3	526·6144	4·319D + 04	9	−2	360·5807	4·795D + 03
6	4	526·6144	4·319D + 04	9	−1	360·5807	4·795D + 03
7	3	531·8334	1·687D + 04	10	−2	368·0397	2·733D + 03
7	2	531·8334	1·687D + 04	10	−3	368·0397	3·029D + 03
8	2	537·7979	9·030D + 03	11	−3	376·2444	1·555D + 03
8	1	537·7979	9·030D + 03	11	−4	376·2444	2·386D + 03

of transition whereas the unprimed parameters correspond to the lower level. The Einstein A-coefficients are used to calculate the mean radiative lifetimes defined by

$$T_{j'\tau'} = 1 \Big/ \sum_{j\tau} A(J'\tau' \to J\tau).$$

The values of the mean radiative lifetimes of the levels are given in table 4.

The Einstein A-coefficients may be used for analysing the spectra of HN_2O^+ from astronomical objects, if observed. Although N_2O has not been detected in the interstellar medium, the calculations by Mitchell [5] have shown that N_2O could be relatively abundant in a shocked intersteller cloud with the speed of the shocks less than 15 km/s. The detection of N_2O however could be difficult because of its very low dipole moment $\mu = 0{\cdot}16$ debye. But the search for the protonated N_2O seems more promising because of its large dipole moment $\mu = 2{\cdot}4$ debye.

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