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Isotopic NS rotational spectra: $^{14}N^{33}S$ and $^{15}N^{32}S$

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Abstract

The mm-wave spectra of the NS radical isotopomers $^{14}N^{33}S$ and $^{15}N^{32}S$ have been measured. Furthermore, new lines of the $^{14}N^{34}S$ species have been recorded. The radicals were generated in a dc glow discharge of a mixture of N_2 and H_2S. All new lines belong to the $^2\Pi_{1/2}$ substates and were observed in natural abundance. The new data have been fitted simultaneously together with previously reported $^{14}N^{32}S$ and $^{14}N^{34}S$ lines to yield molecular constants, including the Born–Oppenheimer corrections Δ_{01}^{S} and Δ_{01}^{N} and the ^{33}S hyperfine constants d and $a-(b+c)/2$.

1. Introduction

The NS radical is a molecule of interest to laboratory as well as interstellar spectroscopy [1]. Rotational spectra of $^{14}N^{32}S$ and $^{14}N^{34}S$ have been reported from laboratory measurements [1–4] including excited vibrational states for the main isotopomer [4]. $^{14}N^{32}S$ has also been detected in interstellar matter in different sources [5–7]. The interest of radio astronomers for highly accurate rest frequencies have led to a thorough study of the $^{14}N^{32}S$ rotational spectrum [1]. For $^{14}N^{34}S$, less accurate data are available [2,3], and there is only one tentative interstellar detection [8] in Sgr B2. This tentative detection reports an intensity of the $^{14}N^{34}S$ species only about 2.5 times weaker than $^{14}N^{32}S$ in the same source [9], which is ten times stronger than the terrestrial ratio. Thus, although this line is unlikely to be really due to $^{14}N^{34}S$, it shows the astrophysical relevance of accurate rest frequencies also for the isotopomers of NS. So far, other isotopomers such as $^{14}N^{33}S$ and $^{15}N^{32}S$ have not been measured.

In the present work, we have searched for the mm-wave spectra of $^{14}N^{33}S$, $^{15}N^{32}S$ and $^{14}N^{34}S$ in order to supply precise frequencies for the possible astronomical detection of the NS isotopomers, and to determine the molecular parameters with special attention to the Born–Oppenheimer correction parameters and hyperfine constants due to the ^{33}S nucleus in $^{14}N^{33}S$.

2. Hamiltonian

The rovibrational levels of a diatomic molecule have first been studied by Dunham [10], and refinements including corrections to the Born–Oppenheimer approximation have been made by Watson [11,12] and Bunker [13]. For states other than $^1\Sigma$, the situation is more complicated due to additional interactions. For $^2\Sigma$ states, in a study of the rotational spectra of BaCl and BaF, Ryzlewicz et al. [14] have adopted Dunham-type expansions for fine and hyperfine structure constants, including the scaling for different nuclear moments of different isotopes of the same element. Concerning $^2\Pi$ states, Brown and co-workers reported si-

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multaneous fits of IR and FIR-LMR data, covering different isotopomers, for SeH [15], GeH [16], and TeH [17]. Anacona et al. [4] have fitted the rotational spectra in vibrational states $v = 0$–5 of the main isotopomer $^{14}N^{32}S$ employing Dunham-type vibrational expressions for all molecular parameters. Here, we incorporated the known isotopic dependences [18] of the vibrational expansion parameters into the matrix elements from Ref. [19]. To account for the breakdown of the Born–Oppenheimer approximation, we replace B_e by U_{01}/μ following Refs. [20,21]. The hyperfine structure for the second nucleus can be included using the matrix elements for the second nucleus from Ref. [22].

3. Experimental

The apparatus of the mm- and sub-mm-wave spectrometer used to detect the NS isotopomer spectra was the same as for the recent investigation of the main isotopomer [1] and is described in Ref. [23]. In the course of this experiment, NS has been produced in a glow dc discharge using a mixture of H_2S (30 mTorr) and N_2 (10 mTorr) at a discharge current of 200 mA. The cell was cooled down to about -80°C.

One principal goal in this experiment was to resolve the ^{33}S hyperfine structure (hfs). This had to be achieved without enrichment (natural atomic abundance of ^{33}S: 0.76%), therefore, we first monitored $^{14}N^{34}S$ lines and optimized the conditions. Then, we tried to detect the ^{15}N isotopomer (0.36%), since the hfs pattern could be easily predicted on the basis of the main isotopomer data. These lines already proved to be faint. A major problem at this low signal level was the presence of considerable baseline fluctuations, preventing an appreciation of the full sensitivity of the spectrometer. Therefore, integrations of scans were performed with and without discharge. For moderately long scans, the baseline fluctuations were significantly reduced by subtracting the reference spectrum from the one with discharge. By this it can also be checked whether the lines were generated in the discharge or not. For the weakest transitions, several difference spectra were added. For the transitions higher than 300 GHz, however, the signals were strong enough so that the data needed not to be subjected to such refined treatments. Fig. 1 shows a spectrum of $^{14}N^{33}S$, revealing the ^{33}S hyperfine structure. Altogether, 9 lines were assigned for $^{15}N^{32}S$, 29 features for $^{14}N^{33}S$ and 19 transitions for $^{14}N^{34}S$, all in the $^2\Pi_{1/2}$ substate and covering a range from 158 to 612 GHz.

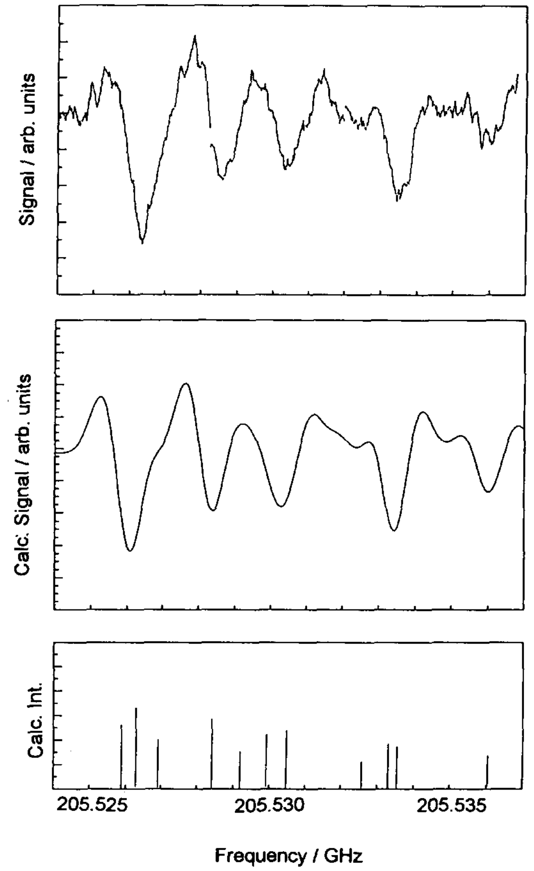

Fig. 1. Observed spectrum of $^{14}N^{33}S(^2\Pi_{1/2})$, together with a calculated spectrum assuming Gaussian profiles for each component. Below, a stick diagram with line positions is given, calculated using the molecular constants from Table 4. The hyperfine pattern belongs to the $J = 4.5 \leftarrow 3.5$ transition in the e parity state.

Tables 1, 2 and 3 comprise the observed frequencies, together with estimates of their uncertainties. The estimates were obtained as follows: We assume a general lower limit of the uncertainty of the system to be about 20 kHz for frequencies up to 400 GHz and 30 kHz for higher frequencies. Whenever a line position was measured several times, we took the statistical error as the uncertainty if the value exceeded the lower limit. For lines measured only once in long integrations, the uncertainty was estimated.

Table 1
$^{15}N^{32}S$: observed transitions (MHz) in the $^2\Pi_{1/2}$ ground state

J'	F'	$\leftarrow$	J''	F''	e/f	ν_{exp}	$\Delta\nu_{exp}$ [a]	Obs.−calc. [b]
4.5	4		3.5	3	e	197902.519	0.100	0.059
4.5	5		3.5	4	e	197904.418	0.100	0.028
4.5	4		3.5	3	f	198279.207	0.100	−0.091
4.5	5		3.5	4	f	198281.948	0.100	0.001
7.5	7		6.5	6	e	329929.480	0.100	0.011
7.5	8		6.5	7	e			
7.5	7		6.5	6	f	330306.351	0.100	−0.143
7.5	8		6.5	7	f	330307.264	0.100	0.001
9.5	9		8.5	8	e	417918.711	0.030	0.028
9.5	10		8.5	9	e			
9.5	9		8.5	8	f	418295.550	0.030	−0.019
9.5	10		8.5	9	f			

[a] Estimated experimental uncertainty. [b] Difference between measured and calculated frequencies. See text for details.

4. Data analysis and discussion

The assignment of the $^{14}N^{34}S$ and $^{15}N^{32}S$ lines did not pose serious problems since their characteristic hyperfine patterns were clearly predictable on the basis of the main isotopomer. Unfortunately, the weakness of the signals, and disturbing lines originating from other molecules prevented us from detecting more transitions, especially the ones covering the $^2\Pi_{3/2}$ state. Thus, the value for the spin–orbit constant and related parameters stem entirely from $^{14}N^{32}S$ data.

Concerning $^{14}N^{33}S$ the situation was far more complicated, due to the unknown hfs of the ^{33}S nucleus. Since especially the lower-J lines were faint, and the hyperfine patterns not completely resolved, a tentative assignment was made by comparing the observed spectra with simulated spectra, covering different values for the hyperfine constants d and $a-(b+c)/2$, but constraining the rotational, fine structure, Λ doubling and ^{14}N hfs parameters to the ones obtained from $^{14}N^{32}S$ and $^{14}N^{34}S$ using reduced-mass dependences. In the next step, the transition frequencies were used in a least-squares fit to give the ^{33}S hyperfine parameters. The overwhelming majority of lines are overlaps of several components, so in the fit, lines were entered as the average of the components, weighted by their calculated intensities. It should be noticed here that the hyperfine interactions of both nuclei are of the same order of magnitude, therefore intensities must be calculated using the eigenvectors obtained in the energy calculation. Finally, the majority of components could be fitted in this way with o–c values below 100 kHz, and observed and calculated spectra show good agreement as can be seen in Fig. 1.

The new data for the three isotopomers measured here were used in a least-squares fit, together with the $^{14}N^{32}S$ $v=0$ data from Lee et al. [1], the $^{14}N^{32}S$ $v=1$–5 transitions from Anacona et al. [4], and the $^{14}N^{34}S$ $v=0$ transitions from Lovas and Suenram [3]. Since no IR data are included, A_{eff} and the vibrational expansion term α_A were constrained to the values adopted in Ref. [4]. The global fit included 232 lines, weighted by the inverse square of their estimated experimental uncertainty, as given in Refs. [3,4]. The frequencies given in Ref. [1] were assumed to have a general uncertainty of 20 kHz. The estimated experimental uncertainties of the present transitions are taken as given in Tables 1–3. Overlapping lines were dealt with as in the respective original references. In coherence with Ref. [1], for the newly measured transition we fitted the sum of the overlapping components, weighted by their calculated intensities, to the observed frequencies.

Table 4 shows the obtained constants; the σ value of the fit was 37 kHz. The Born–Oppenheimer equilibrium bond distance is also given, as well as the correction parameters Δ_{01}^{N} and Δ_{01}^{S}. The vibrational expansion coefficients agree well with the values obtained in Ref. [4], whereas the Λ doubling constants agree rather with Lee's values. Except for eQq_2, not found to be significant here, the present ^{14}N parameters agree well with the data from Ref. [1].

Table 2
$^{14}N^{33}S$: observed transitions (MHz) in the $^2\Pi_{1/2}$ ground state

J'	F_1'	F'	$\leftarrow$	J''	F_1''	F''	e/f	ν_{exp}	$\Delta\nu_{exp}$ [a]	Obs.−calc. [b]
3.5	5	6		2.5	4	5	e	159807.695	0.100	−0.035
3.5	4	5		2.5	3	4	e			
3.5	3	4		2.5	2	3	e	159809.480	0.200	−0.015
3.5	5	5		2.5	4	4	e	159811.330	0.100	−0.053
3.5	4	4		2.5	3	3	e	159814.595	0.100	0.062
3.5	5	4		2.5	4	3	e			
3.5	5	6		2.5	4	5	f	160210.040	0.150	0.102
3.5	5	5		2.5	4	4	f	160211.230	0.150	0.054
3.5	5	4		2.5	4	3	f	160212.515	0.150	0.143
3.5	2	1		2.5	1	1	f			
3.5	4	3		2.5	3	2	f	160222.488	0.200	0.027
3.5	4	4		2.5	3	3	f	160225.117	0.200	0.151
4.5	5	6		3.5	4	5	e	205526.216	0.200	−0.095
4.5	6	7		3.5	5	6	e			
4.5	4	5		3.5	3	4	e			
4.5	6	6		3.5	5	5	e	205528.438	0.100	0.010
4.5	5	5		3.5	4	4	e	205530.231	0.100	0.039
4.5	6	5		3.5	5	4	e			
4.5	5	4		3.5	4	3	e	205533.363	0.100	−0.013
4.5	4	4		3.5	3	3	e			
4.5	4	3		3.5	3	2	e	205535.794	0.100	−0.192
4.5	6	7		3.5	5	6	f	205925.486	0.150	−0.059
4.5	6	6		3.5	5	5	f			
4.5	6	5		3.5	5	4	f	205926.576	0.150	−0.078
4.5	5	6		3.5	4	5	f	205936.064	0.100	0.030
4.5	4	4		3.5	3	3	f			
4.5	4	3		3.5	3	2	f			
4.5	4	5		3.5	3	4	f	205942.621	0.200	0.208
5.5	6	7		4.5	5	6	e	251238.994	0.100	0.069
5.5	7	8		4.5	6	7	e			
5.5	5	6		4.5	4	5	e			
5.5	4	4		4.5	3	3	e	251243.435	0.100	0.069
5.5	6	5		4.5	5	4	e			
5.5	5	5		4.5	4	4	e			
5.5	5	4		4.5	4	3	e	251245.334	0.150	0.066
5.5	6	5		4.5	5	4	f	251641.131	0.150	−0.027
5.5	6	6		4.5	5	5	f			
5.5	6	7		4.5	5	6	f	251642.961	0.150	0.084
5.5	5	5		4.5	4	4	f			
5.5	5	4		4.5	4	3	f			
5.5	4	3		4.5	3	2	f	251645.084	0.200	−0.168
5.5	5	6		4.5	4	5	f	251646.546	0.100	−0.088
5.5	4	4		4.5	3	3	f	251647.942	0.100	0.049
5.5	4	5		4.5	3	4	f			
9.5	11	12		8.5	10	11	f	434421.586	0.043	0.041
9.5	11	11		8.5	10	10	f			
9.5	11	10		8.5	10	9	f			

Table 2
Continued

J'	F_1'	F'	←	J''	F_1''	F''	e/f	ν_{exp}	$\Delta\nu_{\mathrm{exp}}$ [a]	Obs.−calc. [b]
9.5	10	9		8.5	9	8	f	434423.796	0.065	−0.086
9.5	10	10		8.5	9	9	f			
9.5	10	11		8.5	9	10	f			
9.5	9	8		8.5	8	7	f			
9.5	9	9		8.5	8	8	f			
9.5	8	7		8.5	7	6	f			
9.5	9	10		8.5	8	9	f			
9.5	8	9		8.5	7	8	f			
9.5	8	8		8.5	7	7	f			

[a] Estimated experimental uncertainty. [b] Difference between measured and calculated frequencies. See text for details.

Table 3
$^{14}N^{34}S$: newly observed transitions (MHz) in the $^2\Pi_{1/2}$ ground state

J'	F'	←	J''	F''	e/f	ν_{exp}	$\Delta\nu_{\mathrm{exp}}$ [a]	Obs.−calc. [b]
3.5	4.5		2.5	3.5	e	158426.983	0.020	−0.009
3.5	3.5		2.5	2.5	e	158428.161	0.020	−0.005
3.5	2.5		2.5	1.5	e	158431.459	0.040	−0.062
3.5	4.5		2.5	3.5	f	158820.003	0.020	0.082
3.5	3.5		2.5	2.5	f	158826.180	0.100	0.117
3.5	2.5		2.5	1.5	f	158826.670	0.200	−0.007
4.5	5.5		3.5	4.5	f	203744.950	0.020	0.068
4.5	4.5		3.5	3.5	f	203745.440	0.033	−0.035
4.5	3.5		3.5	2.5	f	203747.548	0.020	−0.013
5.5	6.5		4.5	5.5	e	249058.609	0.020	0.017
5.5	5.5		4.5	4.5	e			
5.5	6.5		4.5	5.5	f	249449.432	0.020	0.031
5.5	5.5		4.5	4.5	f	249451.630	0.020	0.044
5.5	4.5		4.5	3.5	f			
7.5	8.5		6.5	8.5	e			
7.5	7.5		6.5	7.5	e	339670.463	0.025	−0.177
7.5	6.5		6.5	6.5	e			
7.5	8.5		6.5	7.5	f	340060.050	0.020	−0.048
7.5	7.5		6.5	6.5	f	340061.137	0.020	0.001
7.5	6.5		6.5	5.5	f			
9.5	10.5		8.5	9.5	e			
9.5	9.5		8.5	8.5	e	430256.940	0.030	0.066
9.5	8.5		8.5	7.5	e			
9.5	10.5		8.5	9.5	f			
9.5	9.5		8.5	8.5	f	430645.865	0.043	0.012
9.5	8.5		8.5	7.5	f			
13.5			12.5		e	611327.524	0.030	0.002
13.5			12.5		f	611713.668	0.030	−0.023

[a] Estimated experimental uncertainty. [b] Difference between measured and calculated frequencies. See text for details.

Table 4
Molecular constants (MHz) for the NS molecule obtained in the present study [a]

Parameter	This work [a]	Ref. [4] [a]	Ref. [1] [a]
U_{01}^{e}	226405.881 (82)		
U_{01}^{N}	30.36 (60)		
U_{01}^{S}	11.09 (37)		
U_{01}^{BO}	226447.339 [b] (141)		
Δ_{01}^{N}	−3.423 [b] (68)		
Δ_{01}^{S}	−2.856 [b] (96)		
Y_{11}	−188.393 (21)	−188.3874 (189)	
Y_{21}	−0.1644 (102)	−0.1671 (84)	
Y_{31}	−0.01256 (128)	−0.01226 (105)	
Y_{02}	0.0376900 (105)	0.037901 (153)	0.0376587 (191)
A_e	6696434 [c]	6696434 [d]	6689869 [d]
α_A	−5585 [c]	−5585 [d]	
$A_{D,e}$	5.1472 (38)	5.1308 (138)	5.06788 [e] (148)
α_{A_D}	−0.2907 (57)	−0.29338 (522)	
p_e	398.630 (111)	396.56 (54)	398.916 [e] (62)
α_p	0.637 (146)	0.593 (129)	
β_p	−0.078 (31)	−0.0748 (256)	
p_D	−0.00813 (36)		−0.00814 (35)
q	−0.680 (42)	0.366 (285)	−0.684 (27)
$h_{1/2}$ (^{14}N) [f]	67.590 (74)	67.645 (99)	67.631
$h_{3/2,e}$ (^{14}N) [g]	57.73 (23)	56.87 (25)	57.548 [e] (52)
$\alpha_{h_{3/2}}$ (^{14}N)	−0.65 (38)	−0.228 (243)	
b (^{14}N)	37.14 (114)	39.8 (57)	37.72 (77)
d (^{14}N)	87.042 (47)	86.953 (81)	87.012 (30)
eqQ_1(^{14}N)	−2.530 (44)	−0.678 (36)	−2.515 (30)
eqQ_2(^{14}N)		−5.8 (33)	−3.30 (151)
$h_{1/2}$ (^{33}S) [f]	125.7 (33)		
d (^{33}S)	124.1 (21)		
r_e^{BO} [b]	1.4939121 (13) Å		

[a] Atomic masses and nuclear magnetic moments for isotopomer scaling were taken from Ref. [24]. Values in brackets: 3σ.
[b] Derived value. [c] Fixed to the value used by Ref. [4]. [d] Fixed. [e] $v = 0$ value. [f] $a - (b + c)/2$. [g] $a + (b + c)/2$.

The determination of the hfs due to the ^{33}S nucleus in $^{14}N^{33}S$ was aggravated by the fact that the lowest rotational transitions could not be measured for being too weak. As a consequence, we failed to find significant values for the electric quadrupole hfs constants eQq_1 and eQq_2.[2] Thus, the dominant contribution to the hfs is magnetic. As with the eQq, a significant value could not be obtained for b.[3] Furthermore, since only the $^2\Pi_{1/2}$ state has been observed in the present investigation, the combination $a + (b+c)/2$ cannot be easily determined. Thus, our experimental data only yielded the magnetic hyperfine constants $a - (b+c)/2$ and d; their values are given in Table 4.

It should be mentioned that the calculated frequencies obtained from the global fit agree similarly well with the observed frequencies as in the references from where they are taken. This indicates that both the vibrational and isotopic dependences are well captured by Dunham-type expansions for all molecular parameters. In particular, the constants for the newly measured isotopomers can be given to a higher accuracy from the global fit; they are tabulated in Table 5.

The global fit reveals a significant deviation from the Born–Oppenheimer approximation as expressed by the correction parameters Δ_{01}^{N} and Δ_{01}^{S} given in

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[2] The fit yielded: $eQq_1 = 0.5(86)$ MHz, $eQq_2 = -61(73)$ MHz, where the values in brackets are 1σ, and b has been fixed to zero.

[3] The fit yielded 10(9) MHz with both eQq's fixed to zero.

Table 5
NS: ground state parameters (MHz) for the measured isotopomers, obtained from the global fit [a]

Parameter	Nucleus	$^{14}N^{33}S$ [a]	$^{14}N^{34}S$ [a]	$^{15}N^{32}S$ [a]
$A_{\rm eff}$		6693683.2 [b]	6693695.3 [b]	6693375.0 [b]
A_D		4.9571 (47)	4.9143 (47)	4.7746 (45)
$B_{\rm eff}$		22942.1189 (135)	22741.9395 (134)	22087.3974 (128)
D		0.036997 (10)	0.036353 (10)	0.034286 (10)
p		395.245 (131)	391.787 (129)	380.483 (126)
p_D		−0.00798 (35)	−0.00784 (35)	−0.00740 (33)
q		−0.668 (41)	−0.656 (40)	−0.619 (38)
$a-(b+c)/2$	$^{14/15}N$	67.590 (74)	67.590 (74)	−94.812 (130)
$a+(b+c)/2$	$^{14/15}N$	57.412 (100)	57.413 (100)	−80.54 (25)
b	$^{14/15}N$	37.14 (114)	37.14 (114)	−52.10 (201)
d	$^{14/15}N$	87.042 (48)	87.042 (48)	−122.099 (42)
eQq_1	^{14}N	−2.530 (44)	−2.530 (44)	
$a-(b+c)/2$	^{33}S	125.7 (33)		
d	^{33}S	124.1 (21)		

[a] Atomic masses and nuclear magnetic moments for isotopomer scaling were taken from Ref. [24]. Values in brackets: 3σ.
[b] Calculated from values adopted by Ref. [4].

Table 4. The Born–Oppenheimer correction parameters have the order of magnitude expected from other molecules; the Δ_{01}^{N} value is 50% larger than in NO, whereas the Δ_{01}^{S} value is 20 % larger than Δ_{01}^{O} in NO [22]. Following the discussion by Watson [12], this may the indicate rovibronic interactions with nearby electronic states to be slightly larger in the ground state of NS than in NO.

5. Concluding remarks

The present study has led to the determination of molecular parameters for the NS radical by a simultaneous fit of all presently available rotational spectra of the different isotopomers. The observed transitions for all isotopomers are well reproduced from the obtained constants. The isotopic dependence of the rotational constant reveals a deviation from the Born–Oppenheimer approximation of the same order as found for other diatomic molecules. The first observation of the ^{33}S hyperfine structure in NS enabled us to determine two magnetic hyperfine constants. Finally, improved frequency predictions of interest to radio astronomy are made possible by the new molecular constants.

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