Radio emission of the interstellar NS molecule

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The frequencies ν and probabilities *A* of radiative transitions between the Λ-doublet levels and the lower rotational levels of the NS molecule, which has recently been detected in the interstellar medium, are calculated. The optical depths and the possibilities of observations of different NS lines in the emission of Sgr B2 are estimated.

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The interstellar NS molecule, which has recently been detected in the radio emission of Sgr B2 (Refs. 1, 2) is of great interest for the chemistry of the interstellar medium. The total number of NS molecules along the line of sight ($nl \approx 10^{14}$ cm^{-2}) proved to be comparable with the number of SO molecules ($5 \cdot 10^{14}$ cm^{-2}). This is in qualitative agreement with the estimates of Oppenheimer and Dalgarno,[3] who predicted the existence of these molecules in the interstellar medium. In doing this they assumed that NS molecules are formed through the reactions $SO + N \rightarrow SN + O$ and $SN^+ + Mg \rightarrow SN + Mg^+$, as well as $SH + N \rightarrow SN + H$, and are destroyed mainly through collisions with N, O, and C^+.

Additional observations in other lines are required for a more exact estimate of the abundance of these molecules and to clarify the possible pumping mechanisms and the populations of their levels. For this one must know the frequencies and probabilities of all the possible transitions.

A diagram of the lower energy levels of the NS molecule is presented in Fig. 1. The electronic ground state $^2\Pi$ of the molecule has two rotational bands $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$. Each rotational level is split into two sublevels of opposite parity: the Λ-doublets. The Λ-splitting for the levels J = 3/2 and J = 5/2 of the $^2\Pi_{3/2}$ band is very small and lies at the limits of error of the experimental measurements. The superfine interaction (magnetic and quadrupole) additionally splits each level of the Λ-doublet in the case of $N^{14}S^{32}$ into three sublevels characterized by the molecule's total angular momentum F = J + 1, J, J − 1.

In Tables I, II, and III we present the calculations which we made of the frequencies ν in MHz, the relative line strengths S divided by the square of the dipole moment, and the Einstein coefficients A in sec^{-1} correspond-

TABLE I. Calculated Frequencies ν, Line Strengths S, and Probabilities A of Spontaneous Transitions between Λ-Doublet levels of $^2\Pi_{1/2}$ Band

$J'F'\pi' \rightarrow JF\pi$		ν, MHz	S/d^2	$A_{J'F'\pi' \rightarrow JF\pi} \times 10^{12}$, sec^{-1}
$^1/_2\,^1/_2-$	$^1/_2\,^1/_2+$	281.28	0.074	0.031
$^3/_2-$	$^1/_2+$	435.76	0.593	0.935
$^1/_2-$	$^3/_2+$	300.86	0.593	0.154
$^3/_2-$	$^3/_2+$	455.34	0.740	0.667
$^3/_2\,^1/_2+$	$^3/_2\,^1/_2-$	678.59	0.222	0.441
$^3/_2+$	$^1/_2-$	725.58	0.158	0.390
$^1/_2+$	$^3/_2-$	701.23	0.158	0.214
$^3/_2+$	$^3/_2-$	748.22	0.430	0.573
$^5/_2+$	$^3/_2-$	829.15	0.192	0.294
$^3/_2+$	$^5/_2-$	783.34	0.192	0.232
$^5/_2+$	$^5/_2-$	864.27	1.001	1.380
$^5/_2\,^3/_2-$	$^5/_2\,^3/_2+$	1087.52	0.096	1.180
$^5/_2-$	$^3/_2+$	1133.11	0.018	0.243
$^3/_2-$	$^5/_2+$	1116.53	0.018	0.169
$^5/_2-$	$^5/_2+$	1162.12	1.345	1.340
$^7/_2-$	$^5/_2+$	1227.47	0.111	1.230
$^5/_2-$	$^7/_2+$	1202.22	0.111	0.988
$^7/_2-$	$^7/_2+$	1266.56	0.210	2.040
$^7/_2\,^5/_2+$	$^7/_2\,^5/_2-$	1490.71	0.088	1.840
$^7/_2+$	$^5/_2-$	1535.44	0.140	3.130
$^5/_2+$	$^7/_2-$	1522.45	0.140	2.410
$^7/_2+$	$^7/_2-$	1567.17	4.009	73.600
$^9/_2+$	$^7/_2-$	1626.92	0.070	1.390
$^7/_2+$	$^9/_2-$	1606.93	0.070	1.160
$^9/_2+$	$^9/_2-$	1666.67	1.359	23.980

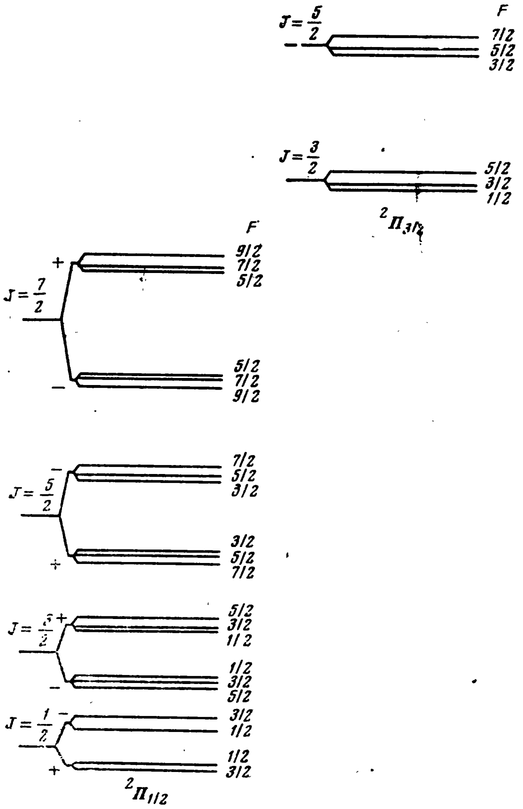

FIG. 1. Diagram of levels of the NS molecule.

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TABLE II. Calculated Frequencies ν, Line Strengths S, and Probabilities A of Spontaneous Transitions between Rotational Levels of $^2\Pi_{1/2}$ Band

$J'F'\pi' \to JF\pi$		ν, MHz	S/d^2	$A_{J'F'\pi' \to JF\pi} \times 10^8$, sec^{-1}
$^3/_2\ ^1/_2-$	$^1/_2\ ^1/_2+$	69040.32	0.593	3.720
$^1/_2+$	$^1/_2-$	69437.63	0.593	3.780
$^3/_2-$	$^1/_2+$	69017.68	0.740	2.320
$^3/_2+$	$^1/_2-$	69484.62	0.740	2.370
$^1/_2-$	$^3/_2+$	69059.98	0.037	0.232
$^1/_2+$	$^3/_2-$	69283.15	0.037	0.234
$^3/_2-$	$^3/_2+$	69037.26	0.593	1.860
$^3/_2+$	$^3/_2-$	69330.24	0.593	1.880
$^5/_2-$	$^3/_2+$	69002.14	2.000	4.180
$^5/_2+$	$^3/_2-$	69411.07	2.000	4.250
$^5/_2\ ^3/_2+$	$^3/_2\ ^1/_2-$	115160.42	1.200	17.480
$^3/_2-$	$^1/_2+$	115573.47	1.200	17.660
$^3/_2+$	$^3/_2-$	115187.18	0.372	5.600
$^3/_2-$	$^3/_2+$	115526.48	0.372	5.640
$^5/_2+$	$^3/_2-$	115158.17	2.020	19.570
$^5/_2-$	$^3/_2+$	115571.69	2.020	19.780
$^3/_2+$	$^5/_2-$	115222.30	0.016	0.233
$^3/_2-$	$^5/_2+$	115445.55	0.016	0.235
$^5/_2+$	$^5/_2-$	115193.29	0.372	3.730
$^5/_2-$	$^5/_2+$	115491.14	0.372	3.760
$^7/_2+$	$^5/_2-$	115154.19	3.200	23.300
$^7/_2-$	$^5/_2+$	115556.48	3.200	23.540
$^7/_2\ ^5/_2-$	$^5/_2\ ^3/_2+$	161305.50	2.286	60.980
$^5/_2+$	$^3/_2-$	161708.71	2.286	61.440
$^5/_2-$	$^5/_2+$	161334.51	2.350	62.760
$^5/_2+$	$^5/_2-$	161624.65	2.350	63.100
$^7/_2-$	$^5/_2+$	161302.78	4.410	88.200
$^7/_2+$	$^5/_2-$	161707.84	4.410	88.870
$^5/_2-$	$^7/_2+$	161373.61	0.008	0.218
$^5/_2+$	$^7/_2-$	161597.77	0.008	0.219
$^7/_2-$	$^7/_2+$	161341.88	0.274	5.480
$^7/_2+$	$^7/_2-$	161642.49	0.274	5.510
$^9/_2-$	$^7/_2+$	161302.12	4.280	68.600
$^9/_2+$	$^7/_2-$	161702.24	4.280	69.120

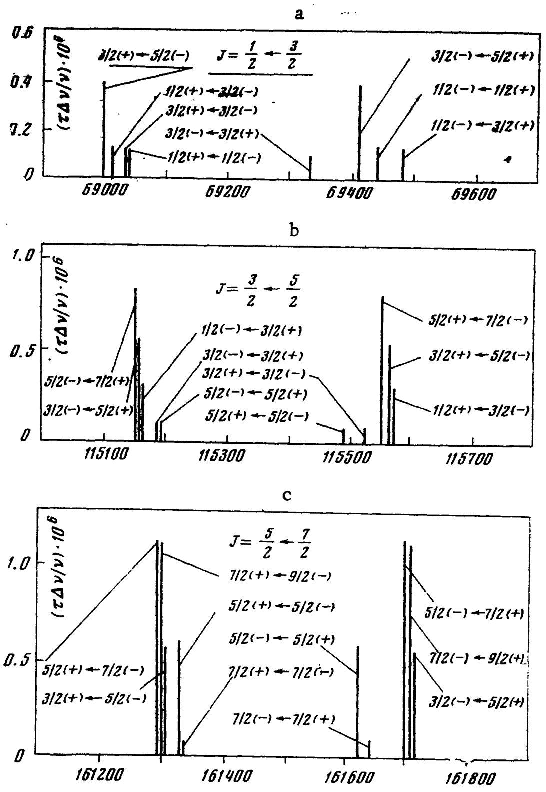

FIG. 2. Optical depths τ multiplied by relative linewidth $\Delta\nu/\nu$ for the superfine components a) J = 1/2←3/2; b) J = 3/2←5/2; c) J = 5/2←7/2 of the $^2\Pi_{1/2}$ band at T = 20°K.

TABLE III. Calculated Frequencies ν, Line Strengths S, and Probabilities A of Spontaneous Transitions between Rotational Levels of $^2\Pi_{3/2}$ Band

$JF'\pi' \to JF\pi$		ν, MHz	S/d^2	$A_{J'F'\pi' \to JF\pi} \times 10^6$, sec^{-1}
$^5/_2\ ^3/_2-$	$^3/_2\ ^1/_2+$	116216.52	0.800	11.970
$^3/_2-$	$^3/_2+$	116181.42	0.256	3.830
$^5/_2-$	$^3/_2+$	116205.49	1.344	13.410
$^3/_2-$	$^5/_2+$	116125.52	0.011	0.159
$^5/_2-$	$^5/_2+$	116149.59	0.256	2.550
$^7/_2-$	$^5/_2+$	116183.86	2.133	15.950

ing to them for transitions within the Λ-doublets of the lower rotational levels J = 1/2, 3/2, 5/2, and 7/2 of the $^2\Pi_{1/2}$ band (Table I) and for transitions between neighboring rotational levels J' → J = 3/2 → 1/2, 5/2 → 3/2, and 7/2 → 5/2 in the band (Table II) and J' → J = 5/2 → 3/2 in the $^2\Pi_{3/2}$ band (Table III). Spectroscopic constants taken mainly from Ref. 4 were used in the calculation. In contrast to Ref. 4, however, the constant of the spin-orbital interaction was taken as equal to 223 cm^{-1}, which leads to better agreement with the experimental frequencies. The relative error of the frequencies presented in Tables I, II, and III is $\delta\nu/\nu \leqslant 10^{-5}$ while that of the line strengths and transition probabilities is $\sim 10^{-2}$–10^{-3}.

The observation of the transition J = 5/3 → 3/2 of the $^2\Pi_{1/2}$ band in Sgr B2 showed that the ratios of intensities of the superfine components of this multiplet are close to the values which should be expected for an optically thin medium in the presence of local thermodynamic equilibrium. If one assumes on this basis that all the rotational levels considered here are thermalized (T ≃ 20°K, Refs. 1 and 2) then one can estimate the optical depths of the calculated radio transitions.

The values of the quantity $\tau\Delta\nu/\nu$, which represents the product of the optical depth times the relative width of the lines, for Sgr B2 are indicated in Fig. 2. It is seen from the figure that the lines which were observed (Fig. 2b) are not the strongest. More substantial emission details should evidently be observed for the transition J = 7/2 → 5/2 (Fig. 2c) near frequencies of 161,300 and 161,707 MHz. They are due to the superposition of the lines F = 5/2(−) → 3/2(+), F = 7/2(−) → 5/2(+), and F = 9/2(−2) → 7/2(+) and of the lines F = 5/2(−) → 3/2(−), F = 7/2(+) → 5/2(−), and F = 9/2(+) → 7/2(−), respectively, since the frequency differences between these superfine transitions lie within the limits of the linewidths, which are much greater than the Doppler width, as follows from the observations of the multiplet J = 5/2 → 3/2.

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