

NH₃, v = 0

Ammonia, v = 0

Species tag	017506
Version	1*
Date of Entry	Dec. 2020
Contributor	H. S. P. Müller

This entry only deals with transitions of ammonia in its ground vibrational state for which ¹⁴N and potentially even ¹H hyperfine structure splitting may be resolved in astronomical sources. The entry is based on preparatory work for (1) S. Yu, J. C. Pearson, B. J. Drouin, K. Sung, O. Pirali, M. Vervloet, M.-A. Martin-Drumel, C. P. Endres, T. Shiraishi, K. Kobayashi, and F. Matsushima, 2010, *J. Chem. Phys.* **133**, Art. No. 174317; which led to versions 5 of ammonia in v = 0 and v₂ = 1 of the JPL catalog from Sep. 2010 with tags 017002 and 017004, respectively. Additional information on this data set was given by (2) B. J. Drouin, S. Yu, and J. C. Pearson, contribution TC 10 presented at the 65th International Symposium on Molecular Spectroscopy, Columbus, OH, USA, June 21–25, 2010. The experimental ground state inversion frequencies with HFS splitting were taken from (3) S. G. Kukolich, 1967, *Phys. Rev.* **156**, 83; for *J_K* = 1₁, 2₂, 3₃, and 3₂. (4) S. G. Kukolich and S. C. Wofsy, 1970, *J. Chem. Phys.* **52**, 5477; for 2₁, 3₁, 4₂, 4₄, and 5₅. (5) S. G. Kukolich, 1965, *Phys. Rev.* **138**, A 1322; for 3₂. (6) D. J. Ruben and S. G. Kukolich, 1974, *J. Chem. Phys.* **61**, 3780; for 5₃. The ground state rotation-inversion transition was reported by (7) G. Cazzoli, L. Dore, and C. Puzzarini, 2009, *Astron. Astrophys.* **507**, 1707. The number of parameter was substantially reduced for the present entry. Most notably, two sets of decic and dodecic parameters were reduced to one each because for the pure inversion transitions only differences in the spectroscopic parameters can be determined. The number of ground state quadrupole distortion parameters and their magnitudes are too large. However, no quick solution was found, and the parameters were retained. Instead, it is recommended to view the calculations with caution for *J* or *K* above 3. The quantum numbers for the regular entry are *J*, *K*, v, and *F*, as usual; v = 0 stands for 0⁺ (or v_t = 0; v = 1 stands for 0[−] (or v_t = 1. *F* includes here the ¹⁴N spin. ¹H hyperfine splitting may matter in astronomical observations. Therefore, a [separate hyperfine calculation](#) is provided for *J* ≤ 6 below 26 GHz. The quantum numbers here are *J*, *K*, v, *n*, and *F*; where *n* is an aggregate spin number that can be disentangled using the part of the out file that is provided. Please note that *F*, the total spin, now including those of the H nuclei, was rounded up to the next integer. **NOTE:** The partition function **does** take into account the spin multiplicity of the ¹H nuclei ! A separate hyperfine calculation with [seven quantum numbers](#) is also available. The quantum numbers in this case are *J*, *K*, v, *F*₁, *F*₂, *I*_{tot}, and *F*; where *F*₁ includes the ¹⁴N spin, *F*₂ is redundant and maybe not meaningful, but needed in the program, *I*_{tot} is the total spin of the hydrogen nuclei rounded up to the next digit, and *F* as above. The dipole moment and its first order distortion corrections were taken from (7) K. Tanaka, H. Ito, and T. Tanaka, 1987, *J. Chem. Phys.* **87**, 1557.

Lines Listed	346
Frequency / GHz	< 3594
Max. <i>J</i>	6
log STR0	-10.0
log STR1	-6.0
Isotope Corr.	-0.0
Egy / (cm ^{−1})	0.0
μ _a / D	
μ _b / D	
μ _c / D	1.4719
<i>A</i> / MHz	10454.260
<i>B</i> / MHz	4041.150
<i>C</i> / MHz	2972.077
Q(300.0)	1766.3450
Q(225.0)	1140.9791
Q(150.0)	623.7662
Q(75.00)	225.4150
Q(50.00)	125.7365
Q(37.50)	84.0965
Q(25.00)	49.2824
Q(18.75)	34.7977
Q(12.50)	22.3963
Q(9.375)	17.2096
Q(5.000)	12.5350
Q(2.725)	12.0104
detected in ISM/CSM	yes

