

Species Tag:	17002	Name:	NH <sub>3</sub>
Version:	5		Ammonia gs inversion
Date:	Spetember 2010		
Contributor:	Shanshan Yu		
	Brian Drouin		
	John Pearson		
Lines Listed:	1716	Q(300.0)=	588.7816
Freq. (GHz) <	20547	Q(225.0)=	380.3263
Max. J:	35	Q(150.0)=	207.9221
LOGSTR0=	-20	Q(75.00)=	75.1383
LOGSTR1=	-20	Q(37.50)=	28.0322
Isotope Corr.:	0.	Q(18.75)=	11.5992
Egy. (cm <sup>-1</sup> ) >	0.0	Q(9.375)=	5.7365
$\mu_a =$	0	A=	B
$\mu_b =$	0	B=	298192.92
$\mu_c =$	1.4719	C=	186695.86

v	state	transition	$\mu_c$
0	gs( <i>s</i> )	gs( <i>a</i> )-gs( <i>s</i> )	1.471932
1	gs( <i>a</i> )	$\nu_2$ ( <i>a</i> )- $\nu_2$ ( <i>s</i> )	1.24478
2	$\nu_2$ ( <i>s</i> )	$\nu_2$ ( <i>s</i> )-gs( <i>a</i> )	0.24725
3	$\nu_2$ ( <i>a</i> )	$\nu_2$ ( <i>a</i> )-gs( <i>s</i> )	0.2363

The Hamiltonian is described in

(1) Yu et al. (J. Chem. Phys. in press)

This entry is a prediction of the ground state inversion transitions only, and the analysis includes hyperfine-free frequencies involving the ground and the  $\nu_2 = 1$  inversion states. A prediction of the  $\nu_2 = 1$  inversion transitions and the  $\nu_2$  fundamental band is given in Entry 17004. The intensities for  $\Delta K=3$  transitions should be viewed with caution, as some  $\Delta K=3$  forbidden transitions were predicted to about 100 times stronger than observed. The  $\Delta K=3$  line intensity has never been studied; the  $\Delta K=3$  Herman-Wallis terms are not known and not included in the intensity calculations. The  $\Delta K=3$  line intensity problem is still under investigation. To avoid confusion, all the unobserved  $\Delta K=3$  transitions were manually removed.

Additional Microwave transitions were taken from

- (2) S.G. Kukolich, Phys. Rev. **138**, A1322 (1965).
- (3) S.G. Kukolich, Phys. Rev. **156**, 83 (1967).
- (4) S.G. Kukolich and S.C. Wofsy, J. Chem. Phys. **52**, 5477 (1970).
- (5) R.L. Poynter, R.K. Kakar, Astrophys. J. Suppl. **29**, 87 (1975).
- (6) M. Ouhayoun, C.J. Borde, J. Borde, Mol. Phys. **33**, 597 (1977).
- (7) S.P. Belov, L.I. Gershstein, A.F. Krupnov, A.V. Maslovskji, S. Urban, V. Spirko,

- D. Papousek, *J. Mol. Spectrosc.* **84**, 288 (1980).
- (8) B.V. Sinha, P.D.P. Smith, *J. Mol. Spectrosc.* **80**, 231 (1980).
- (9) P. Minguzzi, M. Tonelli, A. Carrozzi, *J. Mol. Spectrosc.* **96**, 294 (1982).
- (10) G. Magerl, W. Schupita, J.M. Frye, W.A. Kreiner, T. Oka, *J. Mol. Spectrosc.* **107**, 72 (1984).
- (11) K.J. Siemsen, J. Reid, *Optics Lett.* **10**, 594 (1985).
- (12) K. Tanaka, Y. Endo, E. Hirota, *Chem. Phys. Lett.* **146**, 165 (1988).
- (13) P.D.P. Smith, S. Firth and R.W. Davis, *J. Mol. Spectrosc.* **144**, 448 (1990).
- (14) G. Winnewisser, S.P. Belov, T. Klaus, S. Urban, *Z. Naturforsch.* **51a**, 200 (1996).
- (15) H. Fichoux, M. Khelkhal, E. Rusinek, J. Legrand, F. Herlemont, S. Urban, *J. Mol. Spectrosc.* **192**, 169 (1998).
- (16) S.P. Belov, S. Urban, G. Winnewisser, *J. Mol. Spectrosc.* **189**, 1 (1998).
- (17) S. Urban, F. Herlemont, M. Khelkhal, H. Fichoux, J. Legrand, *J. Mol. Spectrosc.* **200**, 280 (2000).
- (18) G. Cazzoli, L.Dore and C. Puzzarini, *Astron. Astrophys.* **507**, 1707 (2009).
- Additional infrared and far-infrared lines were taken from
- (19) S.M. Freund, T. Oka, *Phys. Rev. A* **13**, 2178 (1976).
- (20) J.J. Hillman, T. Kostiuk, D. Buhl, J.L. Faris, J.C. Novaco, M.J. Mumma, *Optics Lett.* **1**, 81 (1977).
- (21) T. Kostiuk, M.J. Mumma, J.J. Hillman, D. Buhl, L.W. Brown, J.L. Faris, *Infrared Phys.* **17**, 431 (1977).
- (22) H. Jones, *Appl. Phys.* **15**, 261 (1978).
- (23) S. Urban, V. Spirko, D. Papousek, R.S. McDowell, N.G. Nereson, S.P. Belov, L.I. Gershtein, A.V. Maslovskij, A.F. Krupnov, J. Curtis, K.N. Rao, *J. Mol. Spectrosc.* **79**, 455 (1980).
- (24) J.P. Sattler, L.S. Miller, T.L. Worchesky, *J. Mol. Spectrosc.* **88**, 347 (1981).
- (25) J. Sattler, T.L. Worchesky, *J. Mol. Spectrosc.* **90**, 297 (1981).
- (26) J.J. Hillman, D.E. Jennings and J.W. Brault, Paper RE 11, 37th Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, 1982.
- (27) R.L. Poynter, J.S. Margolis, *Mol. Phys.* **48**, 401 (1983).
- (28) S. Urban, D. Papousek, J. Kauppinen, K. Yamada, G. Winnewisser, *J. Mol. Spectrosc.* **101**, 1 (1983).
- (29) P. Shoja-Chaghervand, E. Bjarnov, R.H. Schwendeman, *J. Mol. Spectrosc.* **97**, 287 (1983).
- (30) R.L. Poynter, J.S. Margolis, *Mol. Phys.* **51**, 393 (1984).
- (31) L.R. Brown, R.A. Toth, *J. Opt. Soc. Am. B* **2**, 842 (1985).
- (32) J. Hermanussen, A. Bizzarri, G. Baldacchini, *J. Mol. Spectrosc.* **119**, 291 (1986).
- (33) S. Urban, R. DCunha, J. Manheim, K.N. Rao, *J. Mol. Spectrosc.* **118**, 298 (1986).
- (34) Z.P. Chu, L. Chen, P.K. Cheo, *J. Quant. Spectrosc. Rad. Transfer* **51**, 591 (1994).
- (35) M. Fabian, F. Ito, K.M.T. Yamada, *J. Mol. Spectrosc.* **173**, 591 (1995).

The rotational dipoles and their  $J$  and  $K$  dependences were taken from  
(36) Ueda and Iwahori, *J. Mol. Spectrosc.* **116** 191 (1986).  
(37) M. Fabian, K.M.T. Yamada, *J. Mol. Spectrosc.* **198**, 102 (1999).

The partition function includes contributions from the ground and  $\nu_2 = 1$  states and  $J$  up to 35.