Species Tag:	41010	Name:	CH3CN
Version:	2		Acetonitrile
Date:	Mar. 2014		Methyl Cyanide
Contributor:	B.J. Drouin		$\nu_8 = 1$

Lines Listed:	5248	Q(300.0)=	14683.6324
Freq. (GHz) <	1832	Q(225.0)=	8045.2161
Max. J:	99	Q(150.0)=	3807.7474
LOGSTR0=	-12.0	Q(75.00)=	1267.6721
LOGSTR1=	-10.0	Q(37.50)=	449.0825
Isotope Corr.:	0.	Q(18.75)=	164.3173
Egy. (cm^{-1}) >	0.0	Q(9.375)=	64.0956
$\mu_a =$	3.78197	A=	158099.0
$\mu_b =$		B=	9198.9
$\mu_c =$		C=	B

The experimental measurements are from: D. Boucher, J. Burie, J. Demaison, A. Dubrulle, J. Legrand, and B. Segard, 1977, J. Mol. Spect. **64**, 290; A. Bauer and S. Maes, 1969, J. Phys. **30**, 169; S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, J. Chem. Phys. **58**, 3155; S. G. Kukolich, G. Lind, M. Barfield, L. Faehl and J. L. Marshall, 1978, J. Am. Chem. Soc. **100**, 7155; S. G. Kukolich, 1982, J. Chem. Phys. **76**, 97; P. Venkateswarlu, J. G. Baker and W. Gordy, 1961, J. Mol. Spectrosc. **6**, 215. D. Boucher, J. Burie, A. Bauer, A. Dubrulle and J. Demaison, 1980, J. Phys. Chem. Ref. Data **9**, 659; F. S. Pavone, L. R. Zink, M. Prevedelli, M. Inguscio and L. Fusina, 1990, J. Mol. Spectrosc. **144**, 45; W. Chen, R. Bocquet, D. Boucher, J. Demaison and G. Wlodarczak, 1991, J. Mol. Spectrosc. **150**, 470; F. X. Brown, D. Dangoisse, and J. Demaison, 1988, J. Mol. Spectrosc. **129**, 483; R. Bocquet, G. Wlodarczak, A. Bauer and J. Demaison, 1988, J. Mol. Spectrosc. **127**, 382; F. Lewen, S. P. Belov, F. Maiwald, Th. Klaus and G. Winnewisser, 1995, Z. Naturforsch. **50a**, 1182; and J. C. Pearson and H. S. P. Müller, 1996, Astrophys. J. **471**, 1067.

The constants A, DK, HK cannot be determined from the microwave spectra and were fixed to the IR measurements of: R. Anttila, V.-M. Horneman, M. Koivussaari and R. Paso, 1993, J. Mol. Spectrosc. **157**, 198. M. Koivussaari, V.-M. Horneman and R. Anttila, 1992, J. Mol. Spectrosc. **152**, 377.

The dipole moment for the ground state was reported by J. Gadhi, A. Lahrouni, J. Legrand and J. Demaison, 1995, J. Chim. Phys. **92**, 1984. The nu_8 dipole was scaled from the ground state value by the amount in J. K. Messer and J. A. Roerts, 1982, J. Mol. Spectrosc. **96**, 351.

The v quantum numbers assign the following: 0 is the ground state, 1 is the K*l¡0 l doublet of nu_8=1, 2 is the K*l¿/=0 doublet of nu_8=1. The v8=1 (CCN bending) band energy of 365.015965(12) cm^{-1} (Koivusaari *et al.*) has been included

in the calculation. The constants Pz^3 and Pz^5 off diagonal were fixed to the values of Koivusaari *et al.*.

The version 2 catalog is the same Hamiltonian as version 1, except the hyperfine calculation has been removed and a vibrational partition function consistent with the ground state entry was utilized.