

Species Tag:	42006	Name:	C-13-H3CN
Version:	2		Acetonitrile,
Date:	December 2009		¹³ C on methyl isotope
Contributor:	H.S.P.Müller		

Lines Listed:	1636	Q(300.0)=	10418.8811
Freq. (GHz) <	1755	Q(225.0)=	6765.7543
Max. J:	99	Q(150.0)=	3682.5661
LOGSTR0=	-6.5	Q(75.00)=	1302.7260
LOGSTR1=	-7.5	Q(37.50)=	462.3803
Isotope Corr.:	-1.977	Q(18.75)=	169.1645
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	65.9716
μ_a =	3.92197(13)	A=	158099.0
μ_b =		B=	8933.3
μ_c =		C=	B

This entry is a combined CDMS and JPL entry. The latest combined fit has been reported by (1) H. S. P. Müller; B. J. Drouin, and J. C. Pearson, 2009, *Astron. Astrophys.* 506, 1487. This work provides new data between 339 and 1193 GHz. Additional data were taken from (2) J. C. Pearson and H. S. P. Müller, 1996, *Astrophys. J.* 471, 1067; and from (3) J. Demaison, A. Dubrulle, and D. Boucher, 1979, *J. Mol. Spectrosc.* 76, 1. The purely K -dependent terms A and D_K were assumed to agree with that of the main isotopolog, see d041001.cat. The predictions are probably reliable throughout. ¹⁴N hyperfine splitting may be resolvable at low values of J and possibly at the highest K . Therefore, predictions with hyperfine splitting have been provided up to $J'' = 5$ (108 GHz). Note: The partition function does not include the spin-multiplicities of ¹⁴N! Therefore, partition function values have to be multiplied by 3 when considering ¹⁴N hyperfine splitting! Vibrational contributions have not been considered in the calculation of the partition function yet. Rough estimates may be obtained by scaling the respective ground state value with the ratio from the main isotopolog. At low temperatures, it may be necessary to discern between A -¹³CH₃CN and E -¹³CH₃CN. The A state levels are described by $K = 3n$, those of E state by $K = 3n \pm 1$. The nuclear spin-weight ratio is 2 : 1 for A -¹³CH₃CN with $K > 0$ and all other states, respectively. The $J_K = 1_1$ level is the lowest E state level. It is 5.5715 cm⁻¹ above ground. The dipole moment was assumed to agree with that of the main isotopolog, see c041001.cat.