

Species Tag:	42007	Name:	CH3C-13-N
Version:	2		Acetonitrile,
Date:	December 2009		¹³ C on cyanide isotope
Contributor:	H.S.P.Müller		

Lines Listed:	1619	Q(300.0)=	10123.2613
Freq. (GHz) <	1806	Q(225.0)=	6573.8080
Max. J:	99	Q(150.0)=	3578.1185
LOGSTR0=	-6.5	Q(75.00)=	1265.8098
LOGSTR1=	-7.5	Q(37.50)=	449.3016
Isotope Corr.:	-1.977	Q(18.75)=	164.3975
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	64.1267
$\mu_a =$	3.92197(13)	A=	158093.3
$\mu_b =$		B=	9194.35
$\mu_c =$		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 312 and 1192 GHz. Additional data were taken from (2) J. C. Pearson and H. S. P. Müller, 1996, *Astrophys. J.* 471, 1067; from (3) J. Demaison, A. Dubrulle, and D. Boucher, 1979, *J. Mol. Spectrosc.* 76, 1; and from (4) S. G. Kukolich, 1982, *J. Chem. Phys.* 76, 97. The purely K -dependent terms A and D_K were assumed to agree with those 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 $J'' = 5$ (111 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 -CH₃¹³CN and E -CH₃¹³CN. 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 -CH₃¹³CN with $K > 0$ and all other states, respectively. The $J_K = 1_1$ level is the lowest E state level. It is 5.5802 cm⁻¹ above ground. The dipole moment was assumed to agree with that of the main isotopolog, see d041001.cat.