

Species Tag:	43005	Name:	13CH313CN
Version:	1		Acetonitrile,
Date:	December 2009		<sup>13</sup> C <sub>2</sub> isotope
Contributor:	H.S.P.Müller		

Lines Listed:	1256	Q(300.0)=	10425.9080
Freq. (GHz) <	1684	Q(225.0)=	6770.3174
Max. J:	95	Q(150.0)=	3685.0494
LOGSTR0=	-5.5	Q(75.00)=	1303.6039
LOGSTR1=	-6.5	Q(37.50)=	462.6913
Isotope Corr.:	-3.943	Q(18.75)=	169.2778
Egy. (cm <sup>-1</sup> ) >	0.0	Q(9.375)=	66.0155
$\mu_a$ =	3.92197(13)	A=	158099.0
$\mu_b$ =		B=	8927.28
$\mu_c$ =		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 249 and 1139 GHz. The purely  $K$ -dependent terms  $A$  and  $D_K$  were assumed to agree with those of the main isotopolog, see d041001.cat. Predictions with uncertainties larger than 0.5 MHz should be viewed with caution. <sup>14</sup>N 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 <sup>14</sup>N! Therefore, partition function values have to be multiplied by 3 when considering <sup>14</sup>N 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  $A$ -<sup>13</sup>CH<sub>3</sub><sup>13</sup>CN and  $E$ -<sup>13</sup>CH<sub>3</sub><sup>13</sup>CN. 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  $A$ -<sup>13</sup>CH<sub>3</sub><sup>13</sup>CN with  $K > 0$  and all other states, respectively. The  $J_K = 1_1$  level is the lowest  $E$  state level. It is 5.5713 cm<sup>-1</sup> above ground. The dipole moment was assumed to agree with that of the main isotopolog, see d041001.cat.