Species Tag:	53001	Name:	C2H3CN
Version:	4		Acrylonitrile,
Date:	Oct. 2009		ground state, $\nu_{11} = 1$
Contributor:	Z. Kisiel		and $\nu_{15} = 1$
	B. J. Drouin		
Lines Listed:	298330	Q(300.0)=	119380.376
Freq. (GHz) <	2000	Q(225.0)=	68141.227
Max. J:	99	Q(150.0)=	31738.832
LOGSTR0=	-10.0	Q(75.00)=	9958.401
LOGSTR1=	-9.0	Q(37.50)=	3481.779
Isotope Corr.:	0	Q(18.75)=	1232.852
Egy. (cm^{-1}) >	0.0, 239, 340	Q(9.375)=	437.499
μ_a =	3.815	A=	49850.697
μ_b =	0.894	B=	4971.1636
μ_c =		C=	4513.8773

The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, J. Mol. Spect. **41**, 333 and Z. Kisiel, *et al.*, 2009 J. Mol. Spect. *in press.*

The measurements were taken from:

(1) C. C. Costain and B. P. Stoicheff, 1959, J. Chem. Phys. **30**, 777.
(2) M. C. L. Gerry and G. Winnewisser, 1973, J. Mol. Spect. **48**, 1.
(3) M. C. L. Gerry, K. Yamada, and G. Winnewisser, 1979, J. Phys. Chem. Ref. Data **8**, 107.
(4) G. Cazzoli and Z. Kisiel, 1988, J. Mol. Spect. **130**, 303.
(5) M. Stolze and D. H. Sutter, 1985, Z. Naturforsch. **40a**, 998.
(6) J. Demaison, J. Cosléou, R. Bocquet, and A. G. Lesarri, 1994, J. Mol. Spect. **167**, 400.
(7) O. I. Baskakov, S. F. Dyubko, V. V. Ilyushin, M. N. Efimenko, V. A. Efremov, S. V. Podnos, and E. A. Alekseev, (1997) J. Mol. Spect. **179**, 94.
(8) J. M. Colmont, G. Wlodarczk, D. Priem, H. S. P. Müller, E. H. Tien, R. J. Richards, and M. C. L. Gerry, 1997, J. Mol. Spect. **181**.
(9) H. S. P. Müller, A. Belloche, K. M. Menten, C. Comito, and P. Schilke, 2008, J. Mol. Spectrosc. 251 319.
(10) Z. Kisiel, L. Pszczólkowski, B. J. Drouin, C. S. Brauer, S. Yu, J. C. Pearson, 2009, J. Mol. Spect. *in press.*

For the ground vibrational state ^{14}N quadrupole splittings have been fitted where they have been resolved experimentally; see e. g. (5), (7), (8).

The partition function given here includes the spin-multiplicity of the ^{14}N nucleus as well as the two low lying vibrational states.

The dipole moment is from (5). The ground state dipole moment was used for the excited states.

The vibrational states are 0 = ground state, 1 = in plane CCN bend, $v_{11} = 1$, at 239 cm^{-1} and 2 = CCN out of plane bend, $v_{15} = 1$, at 340 cm^{-1}.

A cutoff (described in Kisiel et al for the combined state analysis) was utilized to avoid force fitting lines in $v_{11} = 1$ that are perturbed by the interaction with the state $v_{15} = 1$ above it. Perturbed lines that remain within this cutoff are the reason why the overall unitless standard deviation, σ_{rms}, of the coupled fit is relatively high at 1.6. We note, however, that this fit encompasses all but one of the measured ground state lines at a much more respectable σ_{rms} of 1.25. The single exception is also most probably a typing error in the literature value.

The v_{15} state is unchanged from version 3 since Kisiel et al. did not provide new analysis of this state. High order parameters from the version 3 fit (which had been shared between vibrational states) were defined only for v_{15} and held fixed in the present analysis - this allows the updated states to be changed independently from the non-updated state.

The quadrupole coupling is analyzed simultaneously with the entire data set, but is based on only ground state splittings reported in the literature. The predicted splittings assume no vibrational dependence.