

Species Tag:	69002	Name:	C3H7CN
Version:	1		Butyronitrile or
Date:	Jan. 1996		n-Propyl cyanide,
Contributor:	J. C. Pearson		anti and gauche forms

Lines Listed:	60671	Q(300.0)=	120097.057
Freq. (GHz) <	2000	Q(225.0)=	79160.238
Max. J:	99	Q(150.0)=	41231.375
LOGSTR0=	-10.0	Q(75.00)=	12254.662
LOGSTR1=	-10.0	Q(37.50)=	3632.345
Isotope Corr.:	0.0	Q(18.75)=	1197.204
Egy. (cm ⁻¹) >	0.0, 92	Q(9.375)=	421.579
μ_a =	3.597	A=	23667.8
μ_b =	0.984	B=	2268.1
μ_c =		C=	2153.0

Butyronitrile is found in two conformers anti and gauche. The anti form is denoted by state 0 while the gauche form is state 1. The dipoles and rotational constants given are for the lower energy anti form which is about 92 cm⁻¹ below the gauche form. There is no evidence of the two forms interacting in the ground state. Lines and dipoles were taken from:

E. Hirota, J. Chem. Phys. **37**, 2918 (1962). J. Demaison and H. Dreizler, Z. Naturforsch. **37a**, 199 (1982). G. Wlodarczak, L. Martinache, J. Demaison, K.-M. Marstokk and H. Mollendal, J. Mol. Spect. **127**, 178 (1988). K. Vormann and H. Dreizler, Z. Naturforsch. **43a**, 338 (1988).

The gauche form has the following dipole moments $\mu_a = 3.272\text{D}$ and $\mu_b = 2.139\text{D}$. The quadrupole has been resolved and is presented in Vormann *et al.* and Demaison *et al.*, above. No quadrupole was used in this calculation.