

Species Tag:	51007	Name:	HCCNC-v5
Version:	1		Ethynyl-isocyanide,
Date:	Jan. 1995		$\nu_5$ vibrational state
Contributor:	M. L. Delitsky H. M. Pickett		
Lines Listed:	278	Q(300.0)=	3775.7021
Freq. (GHz) <	985.34	Q(225.0)=	2832.7507
Max. J:	99	Q(150.0)=	1888.7322
LOGSTR0=	-10.0	Q(75.00)=	944.7917
LOGSTR1=	-100.0	Q(37.50)=	472.8781
Isotope Corr.:	0.0	Q(18.75)=	236.9363
Egy. ( $\text{cm}^{-1}$ ) >	634.0	Q(9.375)=	118.9708
$\mu_a =$	2.93	A=	
$\mu_b =$		B=	4970.517
$\mu_c =$		C=	

The observed frequency measurements were taken from A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, J. Mol. Spect. **156**, 39. The  $\nu_5$  vibration is the lowest excited bending state at  $634 \text{ cm}^{-1}$ . It should be noted that the  $\nu_5$  is an  $l$  doubled state.

The dipole moment was assumed to be the same as for the ground state. M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, Angew. Chem. Int. Ed. Engl. **30**, 1644.