

|                            |                |           |            |
|----------------------------|----------------|-----------|------------|
| Species Tag:               | 51004          | Name:     | HCCNC      |
| Version:                   | 1              |           | Ethynyl    |
| Date:                      | Dec. 1994      |           | isocyanide |
| Contributor:               | M. L. Delitsky |           |            |
|                            | H. M. Pickett  |           |            |
| Lines Listed:              | 563            | Q(300.0)= | 3775.7021  |
| Freq. (GHz) <              | 991.05         | 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. (cm <sup>-1</sup> ) > | 0.0            | Q(9.375)= | 118.9708   |
| $\mu_a$ =                  | 2.93           | A=        |            |
| $\mu_b$ =                  |                | B=        | 4967.838   |
| $\mu_c$ =                  |                | C=        |            |

The observed frequency measurements were taken from: A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, *J. Mol. Spect.* **156**, 39. M. Krüger, W. Stahl and H. Dreizler, 1992, *J. Mol. Spect.* **158**, 298. The quadrupole coupling values were investigated in M. Krüger, above. Detailed field gradients and quadrupole coupling constants are presented in D. Cremer and M. Krüger, 1991, *J. Phys. Chem.* **96**, 3239.

The dipole moment was taken from M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, *Angew. Chem. Int. Ed. Engl.* **30**, 1644.