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|---|---|---|---|
| Species Tag: | 41001 | Name: | CH3CN |
| Version: | 4 | | Acetonitrile |
| Date: | Dec. 2009 | | Methyl Cyanide |
| Contributor: | H. S. P. Müller | | g.s. |
| | | | |
| Lines Listed: | 1728 | Q(300.0)= | 10118.2635 |
| Freq. (GHz) < | 1864 | Q(225.0)= | 6570.5621 |
| Max. J: | 99 | Q(150.0)= | 3576.3518 |
| LOGSTR0= | -7.0 | Q(75.00)= | 1265.1853 |
| LOGSTR1= | -8.5 | Q(37.50)= | 449.0803 |
| Isotope Corr.: | 0. | Q(18.75)= | 164.3168 |
| Egy. ($cm^{-1}$) > | 0.0 | Q(9.375)= | 64.0955 |
| $\mu_a$ = | 3.92197(13) | A= | 158099.0 |
| $\mu_b$ = | | B= | 9198.9 |
| $\mu_c$ = | | C= | B |

This entry is a combined CDMS and JPL entry. The $\nu_8$ entry is now a separate catalog entry under 41010. 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 in the 1.58-1.63THz region. Additional, extensive data between 91 and 1192 GHz were published in (2) G. Cazzoli and C. Puzzarini, 2006, *J. Mol. Spectrosc.* **240**, 153. As in that work, additional data were taken from (3) S. G. Kukolich, D. J. Ruben, J. H. S. Wang, and J. R. Williams, 1973, *J. Chem. Phys.* **58**, 3155; from (4) S. G. Kukolich, 1982, *J. Chem. Phys.* **76**, 97; and from (5) D. Boucher, J. Burie, J. Demaison, A. Dubrulle, J. Legrand, and B. Segard, 1977, *J. Mol. Spectrosc.* **64**, 290. The purely $K$-dependent terms were determined through $\Delta K = 3$ infrared loops from (6) R. Anttila, V.-M. Horneman, M. Koivusaari, and R. Paso, 1993, *J. Mol. Spectrosc.* **157**, 198. The predictions should be reliable throught with the exception of $K$ >14 transitions between about $J = 36$ and 48 which are perturbed by a weak resonant interaction with $v_8 = 1$. $^{14}$N hyperfine splitting may be resolvable at low values of $J$ and possibly at the highest $K$. Therefore, predictions with http://spec.jpl.nasa.gov/catalog/hfs/c041001_hfs.cat hyperfine splitting have been provided up to $J$" =9 (184 GHz). The partition function does **not** include the spin-multiplicities of $^{14}$N. Therefore, partition function values have to be multiplied by 3 when considering $^{14}$N hyperfine splitting. Vibrational contributions have been considered in the calculation of the partition function for states up to about 1200 $cm^{-1}$. Higher vibrational states contribute to less than 1% each at 300 K. Values for the ground state are given in parentheses. Additional information on http://www.ph1.uni-koeln.de/site/vorhersagen/daten/CH3CN/CH3CN/CH3CN.Q vibrational states is also available. The dipole moment was determined by (7) J. Gadhi, A. Lahrouni, J. Legrand, and 1995, *J. Chem. Phys.* **92**, 1984.