

Species Tag: 31010 Name: CH₃CH₂D g.s and ν_{18}
 Version: 1 1D-Ethane
 Date: Dec. 2014
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Lines Listed: 38764 Q(300.0)= 32720.6379
 Freq. (GHz) < 2000 Q(225.0)= 18267.0606
 Max. J: 50 Q(150.0)= 8698.1224
 LOGSTR0= -12.0 Q(75.00)= 2858.7608
 LOGSTR1= -12.0 Q(37.50)= 1008.6979
 Isotope Corr.: 0 Q(18.75)= 359.2054
 E_{gy}. (cm⁻¹) > 0.0 Q(9.375)= 128.8711
 μ_a = 0.015 (gs) A= 69653.392
 μ_b = 0.015 B= 18859.082
 μ_c = C= 18214.160

Initial work by E. Hirota, Y. Endo, S. Saito, J.L. Duncan, Microwave spectra of deuterated ethanes: J. Mol. Spectrosc. 89 (1981) 285-295 measured the rotational spectrum in the ground state of CH₃CH₂D up to 160 GHz including 12 pairs of *a*- and 15 pairs of *b*- dipole transitions that were split into two hindered rotation components (*A* and *E*).

Subsequent measurements made at JPL by A.M.Daly, B.J. Drouin, P. Groner, S.Yu and J. C. Pearson (JMS 307, p. 27-32, 2015) report the pure rotational spectrum of the ground and first excited torsional state ν_{18} of CH₃CH₂D, with measurements made up to 1.6 THz for the ground state and 1.1 THz for the ν_{18} state. The energy differences between the *A* and *E* torsional substates, $\Delta E(E-A)$, of 74.167(18) and -3382.23(34) MHz for the ground and excited states, respectively. Using these energy differences and the overtone transitions $\Delta\nu_{18} = 2$ from Raman measurements in the literature J.M. Fernández-Sánchez, S. Montero, J. Chem. Phys. 94 (1991) 7788-7800, the coefficients V_3 and V_6 of the potential function of the internal rotation in CH₃CH₂D were determined as $V_3 = 1004.56(4)$ cm⁻¹ and $V_6 = 7.09(12)$ cm⁻¹.

The dipole moment components are estimated to be equal components of the deuteromethane dipole (J. K. G. Watson, M. Takami, and T. Oka, 1979, J. Chem. Phys., 70, 5376).

	gs	$\nu_{18} = 1$
A	0	3
E	1,2	4,5

The partition function at 300 K was calculated with a sum-over-states up to *J* of 80, and does include other vibrational states below 990 cm⁻¹. The summation is truncated at *J* = 50.