

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_g. (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 in press) 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.