

Species Tag: 48011 Name: CH3OOH
Version: 1 Ground
Date: Dec. 2005 0⁺, 0⁻, A, E States
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Lines Listed: 46191 Q(300.0)= 106466.2980
Freq. (GHz) < 1800 Q(225.0)= 68323.1834
Max. J: 50 Q(150.0)= 36346.9932
LOGSTR0= -11.0 Q(75.00)= 12054.7879
LOGSTR1= -7.0 Q(37.50)= 3811.4277
Isotope Corr.: -0.007 Q(18.75)= 1139.3855
Egy. (cm⁻¹) > 0.0 Q(9.375)= 339.0903
 μ_a = 0.606 / 0.703 A= 42828.738
 μ_b = 0.071 / 0.133 B= 10500.288
 μ_c = 0.5 C= 9055.050

The frequencies and dipole moment were taken from: M. Typlewski, T. -K. Ha, R. Meyer, A. Bauder, C. E. Blom, 1992, J. Chem. Phys. **97**, 9. The 'c' type transition dipole moment is unknown so a 0.5 D dipole was assumed in the calculations. A $K_a = 6 \leftarrow 7$ Q branch between the 0⁺ and 0⁻ states was reassigned for splittings due to methyl torsion (A/E) rather than asymmetry splittings. This results in an improved global fit to the four states.

The state specific quantum numbers, v = 0-5 correspond to the following symmetries:

inversion	<i>I.R.</i>	v
0 ⁺	A	0
0 ⁺	E	1,2
0 ⁻	A	3
0 ⁻	E	4,5