

Species Tag:	32003	Name:	CH3OH
Version:	3		Methyl alcohol,
Date:	March 2010		<i>A, E₁, and E₂</i>
Contributor:	J.C. Pearson		$v_t = 0,1,2$
	L.-H. Xu		
Lines Listed:	83543	Q(300.0)=	9473.1198
Freq. (GHz) <	6000	Q(225.0)=	5267.8635
Max. J:	40	Q(150.0)=	2437.7654
LOGSTR0=	-20	Q(75.00)=	731.0698
LOGSTR1=	-20	Q(37.50)=	230.2391
Isotope Corr.:	0	Q(18.75)=	68.7464
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	19.5433
$\mu_a =$	0.896	A=	127484.
$\mu_b =$	1.412	B=	24679.98
$\mu_c =$		C=	23769.70

This entry is based on a Rho axis method calculation done with the data set described in L.-H. Xu, J. Fisher, R.M. Lees, H.Y. Shy, J.T. Hougen, J.C. Pearson, B.J. Drouin, G.A. Blake, & R. Braakman, 2008, *J. Mol. Spectrosc.* 251, 305. The analysis was an initial global attempt to include $v_t=2$; however, not all the available assignments were included in the analysis so some $v_t=2$ levels are known to be systematically shifted. The shifts affect the b-type rotational and b- and c-type torsional transitions the most. Only data to $J=30$ was included in the analysis so it is known that levels deviate above $J=30$, but the deviations are experimentally known to be both small and smooth. The bands included are manually selected in the program rather than subject to an automatic intensity threshold. As a result, some bands with significant intensity are not included while other very weak bands are included.

This entry has not been merged with measured lines due to a number of known problems in the data set. There is a plan for an improved analysis in the future including transitions through at least $J=40$, however the need to assign Herschel data above 1 THz has made this entry a priority. The $K=0$ A-state transitions were manually corrected to have about the proper intensity, so the intensity should only be trusted at the few percent level on these transitions. Low J ($J < 4$) A-state $\Delta K = 2$ or 3 were deleted since they were predicted to be several orders of magnitude too strong. A number of doubled transitions were manually deleted with no assurance that all were removed. Should any transitions be included twice with the same frequency and quantum numbers there should only be one and the other can be ignored as missed in the editing process. Finally a calculation artifact involving transitions between $J=35$ and $J=36$ was manually corrected. The large uncertainty was left in the prediction as a reminder that the correction was manually done with some uncertainty (300kHz) in the exact magnitude of the calculation error. Uncertainties in the b -type or c -type transitions involving K 's not in the fit should not be trusted.

The following K levels are the largest in the fit $v_t=0$ A-state $K=13$, E-states $K=-13$ and $K=12$, $v_t=1$ A-state $K=12$, E-states $K=-10$ and $K=12$. In $v_t=2$ the following sets of A-state levels were included in the analysis $K=1-0$, $K=3-2$, $K=4-3$, $K=7-6$. The E-states included are $K=-5$ to -4 , $K=-1$ to -2 , $K=0$ to -1 , $K=2-1$, $K=3-2$, $K=5-4$, & $K=6-5$. Predictions of $a-$ type ($\Delta K = 0$) transitions are known to be pretty good for most $K < 11$ $v_t=2$ transitions.

The partition function was calculated as an explicit sum over energy levels generated by this calculation to $J = 44$ and $K = 20$ for $v_t=0,1,2$. The contribution of $v_t=2$ was estimated based on energy levels to $J = 22$ calculated by M.A. Mektiev, P.D. Godfrey, & J.T. Hougen, 1999, *J. Mol. Spectrosc.* 194, 171 scaled by the ratio of $v_t=2$ from $J = 44$ relative to $v_t=2$ $J = 22$. The vibrational partition function for all the other modes was calculated following M. Dang-Nhu, M. Allegrini, & G. Moruzzi, *J. Mol. Spectrosc.* 140, 412 and was used as a multiplier for the torsional manifold to give the full partition function. This is a deviation from the usual approach of just the levels calculated. It should be noted that truncation of the energy levels at $J = 44$ and $K = 20$ will underestimate the partition function at temperatures above 300K. At 300K the error is at most a few out of the 9472. The partition function used ignores spin beyond the A and E states dividing the full partition function by the common factor of 4. If thermodynamic quantities are involved the partition function given here should be multiplied by 4 to include the common spin multiplicity.

The quantum number format is $J, \pm K$, parity (\pm), v_t . A-state transitions have a '+' or '-' in the parity column while E states do not. E1 and E2 are denoted by the positive (unsigned) and negative sign of K , respectively, in the absence of a parity entry.

The dipole moment was taken from K.V.L.N. Sastry, R.M. Lees, & J. Van Der Linde, 1981, *J. Mol. Spectrosc.* 88, 228 and no attempt was made to include any torsional dependence. It is known from ^{13}C and ^{18}O methanol that μ_a increases by about 0.04 Debye with increasing torsional state (not included in calculation). It remains unclear what μ_b does with torsion; however, the torsional overlap rather than the usual asymmetric top direction cosine matrix element dominates the line strengths in $v_t=2$ and above.