Species Tag:	33004	Name:	CH2DOH
Version:	1		Methyl alcohol D1
Date:	July 2012		
Contributor:	J.C. Pearson		Ground e_0, e_1 and o_1
Lines Listed:	89098	Q(300.0)=	15172.
Freq. (GHz) <	6000	Q(225.0)=	9410.3473
Max. J:	40	Q(150.0)=	4359.4672
LOGSTR0=	-20	Q(75.00)=	1292.7487
LOGSTR1=	-20	Q(37.50)=	399.0612
Isotope Corr.:	0	Q(18.75)=	114.5900
Egy. (cm^{-1}) >	0.0	Q(9.375)=	30.3886
μ_a =	0.896	A=	103551.3
μ_b =	1.412	B=	23047.8
μ_c =		C=	21686.5

The calculation is based on the method described in Pearson et al. 2012, Journal of Molecular spectroscopy, in press. DOI 10.1016/j.jms.2012.06.012. Additional data from

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I. Mukhopadhyay, K.V.L.N. Sastry, Spectrochim. Acta A 53 (1997) 2061-2065.

C.F. Su, C.R. Quade, J. Mol. Spectrosc. 134 (1989) 290-296.

M. Liu, C.R. Quade, J. Mol. Spectrosc. 149 (1991) 557-558.

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was used in the analysis. CH_2DOH is an asymmetric top with a ground state comprised of three sub-states e_0, e_1 and o_1. These are denoted with v=0,1,2, respectively. The lower K_a levels are strongly interacting and should not be trusted beyond J=30 where the stated accuracy will be much worst than reality. K_a values to 10,9,9 in v=0,1,2 were connected. Calculated levels with higher K_a value will deviate strongly in the absolute energy. This means any transition changing K_a above K_a=10,9,9 in v=0,1,2 will not be accurate with the exception of the e_1 K_a=11 to o_1 K_a=10 band where the relative energies are correct. The a-type R branches to K=11 were

included in the data and are calculated reasonable well. Because of the poor extrapolative power of the model the accuracy of predictions rapidly deteriorates above 2 THz and for $K_a > 10,9,9$.

The intensites were calculated with the first order Fourier term of the dipole from normal methanol. The strongly allowed bands are reasonably well reproduced, but the weeker ones are not as well re-produced. Extreme caution should be used in determining columns (or concentrations) directly from b-type and c-type transitions as significant errors can occur. The a-type transitions should be much more reliable for column determinations.