

Species Tag:	46004	Name:	C2H5OH
Version:	4		Ethyl alcohol,
Date:	April 2008		<i>trans</i> , <i>gauche</i> states
Contributor:	J. C. Pearson		

Lines Listed:	52180	Q(300.0)=	45583.6606
Freq. (GHz) <	2000	Q(225.0)=	28437.8924
Max. J:	80	Q(150.0)=	14312.2584
LOGSTR0=	-10.0	Q(75.00)=	4106.4006
LOGSTR1=	-8.0	Q(37.50)=	1072.4178
Isotope Corr.:	0.0	Q(18.75)=	290.9463
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	95.5970
μ_a =	0.046	A=	34891.7707
μ_b =	1.462	B=	9350.6776
μ_c =	0.000	C=	8135.2352

Trans State: The experimental measurements were analyzed using the methods described in W. H. Kirchhoff, 1972, *J. Mol. Spect.* **41**, 333. The measurements were taken from: J. Michielson-Effinger, 1969, *J. Phys. (Paris)* **30**, 333, Y. Sasada, M. Takano, and T. Satoh, 1971, *J. Mol. Spect.* **38**, 33, H. Takano, Y. Sasada, and T. Satoh, 1968, *J. Mol. Spect.* **26**, 157, F. J. Lovas, 1982, *J. Phys. Chem. Ref. Data* **11**, 251, and J. C. Pearson, K. V. L. N. Sastry, M. Winnewisser, E. Herbst, and F. De Lucia, 1995, *J. Phys. Chem. Ref. Data* **24**, 1-32. J. C. Pearson, C.S. Brauer & B.J. Drouin, *J. Mol. Spectrosc.*, in press, 2008 The dipole moment was reported by Takano *et al.*, above. The *trans* state transitions are designated as $v = 2$. The dipoles and rotation constants listed are for the *trans* state.

Gauche States: The analysis used here is based on a modified Fixed Frame Axis Method (FFAM) which is described in C. R. Quade and Chun C. Lin, 1963, *J. Chem. Phys.* **38**, 540-550 with the addition of a periodic $\text{Ecos}(pK)$ with equal and opposite signs for the two gauche states. Measurements were taken from: E. A. Cohen, 1979, unpublished, R. K. Kakar and C. R. Quade, 1980, *J. Chem. Phys.* **78**, 4300-4307, and J. C. Pearson, K. V. L. N. Sastry, E. Herbst and F. C. De Lucia, 1995, submitted to *J. Mol. Spect.* J. C. Pearson, K. V. L. N. Sastry, E. Herbst and F. C. De Lucia, 1996, *J. C. Pearson, C.S. Brauer & B.J. Drouin, J. Mol. Spectrosc.*, in press, 2008 The dipole moment was reported by Kakar and Quade, above. The dipoles are $\mu_a = 1.264$, $\mu_b = 0.104$, and $\mu_c = 1.101$. The vibrational quantum number $v = 0$ is used to designate the lower *gauche+* state and $v = 1$ to designate the *gauche-* state.

Both States: The analysis is described in Pearson et al. 2008. It includes both substates as well as several thousand transitions between the two. Intensities were calculated from the fixed dipole moments with no knowledge of the torsional overlaps. It is known that the intensities of A-type Delta K not zero transitions, X-type, and perturbed transitions including almost all trans to gauche can have differences in

intensity from the calculation by an order of magnitude. Fortunately the strongest lines are generally in excellent agreement with the predicted intensities. The existing data effectively ends at $K=26$ and any higher K will be wrong by significantly more than the calculated value. The J range extends to 53 for K_j10 and increases to 71 for K_j4 . Q branches to 76 were in the analysis at $K=0$ and 1.