

Species Tag: 56008 Name: C2H3CHO
Version: 1 s-trans and s-cis Acrolein
Date: Jan. 1996
Contributor: J. C. Pearson

Lines Listed:	24051	Q(300.0)=	25617.3419
Freq. (GHz) <	2000	Q(225.0)=	17407.4359
Max. J:	50	Q(150.0)=	9906.6949
LOGSTR0=	-8.0	Q(75.00)=	3580.8756
LOGSTR1=	-8.5	Q(37.50)=	1267.7973
Isotope Corr.:		Q(18.75)=	449.0120
Egy. (cm ⁻¹) >	0.0, 594	Q(9.375)=	159.3214
μ_a =	3.052	A=	47353.7
μ_b =	0.630	B=	4659.5
μ_c =	0	C=	4242.7

Acrolein exists in two stable conformers, s-trans and s-cis. The s-trans state is more stable by 594 cm⁻¹. The dipole moments and rotational constants given are for the s-trans conformer.

The s-trans experimental measurements were taken from: R. Wagner, J. Fine, J. W. Simmons and J. H. Goldstein, *J. Chem. Phys.* **26**, 634 (1957). E. A. Cherniak and C. C. Costain, *J. Chem. Phys.* **45**, 104 (1966). M. Winnewisser, G. Winnewisser, T. Honda and E. Hirota, *Z. Naturforsch.* **30a**, 1001 (1975).

The dipole moments and measurements for the s-cis state come from: C. E. Blom and A. Bauder, *Chem. Phys. Lett.* **88**, 55 (1982). C. E. Blom, G. Grassi and A. Bauder, *J. Am. Chem. Soc.* **106**, 7427 (1984).

The s-trans levels are denoted as state 0 and s-cis is state 1. The dipole moments for the s-cis form are $\mu_a = 2.010\text{D}$ and $\mu_b = 1.573\text{D}$.

The partition function listed in this file was corrected from erroneous values on October 3rd 2012.