Species Tag:	57003	Species Name:	HCCCH2OD
Version:	1		OD Propargyl Alcohol
Date:	June 2006		Gauche+ and Gauche-
Contributor:	J. C. Pearson		Ground state
Lines Listed:	22458	Q(300.0)=	48293.8475
Freq. (GHz) <	2000	Q(225.0)=	36268.7494
Max. J:	40	Q(150.0)=	22624.4147
LOGSTR0=	-10.0	Q(75.00)=	8556.2144
LOGSTR1=	-7.0	Q(37.50)=	2875.4533
Isotope Corr.:	0	Q(18.75)=	913.1355
Egy. (cm^{-1}) >	0.0	Q(9.375)=	273.9361
μ_a =	1.037	A=	29643.4
μ_b =	0.147	B=	4612.8
μ_c =	0.75	C=	4130.6
		ΔE=	213321.8

The experimental measurements were described in J.C. Pearson and B.J. Drouin, 2005, J. Mol. Spectrosc. 234, 149. The dipole of the OH specicies was assumed for the OD species. The catalog contains the calculated frequencies from a quadratic interaction analysis. The catalog analysis differs from the paper in that the constants that resulted in significant differences between torsional substates were fixed together. This allowed D_{bc} to be determined, but due to lack of real information on the a-type resonance the value is probably not trustworthy.

The data set is quite limited with a few low J ^{a}R branches and a few c-type at low frequency. The poorly determined a-type interaction will strongly affect the asymmetry splitting at low K_a and higher J. As a result the K_a transitions for 0,1,2 will be problematic above J=20. K_a values between 3 and 7 will be some what better possibly to between J=25 and 35. Above K_a=10 there is no data and the calculation is not believable.