

Species Tag:	77003	Name:	C3H8O2 I 13C5
Version:	1		13C5 1,3 propanediol,
Date:	March 2010		
Contributor:	B.J. Drouin		Conformer I
Lines Listed:	11250	Q(300.0)=	76359.5541
Freq. (GHz) <	300	Q(225.0)=	53434.2052
Max. J:	30	Q(150.0)=	31473.7492
LOGSTR0=	-10.0	Q(75.00)=	11875.5875
LOGSTR1=	-10.0	Q(37.50)=	4247.0508
Isotope Corr.:	0.0	Q(18.75)=	1503.5587
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	532.8032
μ_a =	2.917	A=	7664.143
μ_b =	1.465	B=	3844.500
μ_c =	1.024	C=	2827.169

The data set used is from D. F. Plusquellic et al. J. Phys. Chem. A 2009, 113, 12911-12918. The partition function was calculated with a summation over predicted energy levels up to $J = 250$. The dipole moment has been assumed to be identical to the parent isotopolog. The heavy carbon atom is atom number 5 in the atom labeling scheme adopted.