

Species Tag:	77002	Name:	C3H8O2 I 13C4
Version:	1		13C4 1,3 propanediol,
Date:	March 2010		v = 0,1
Contributor:	B.J. Drouin		Conformer I
Lines Listed:	21991	Q(300.0)=	152013.7493
Freq. (GHz) <	300	Q(225.0)=	106460.3637
Max. J:	30	Q(150.0)=	62782.5051
LOGSTR0=	-10.0	Q(75.00)=	23729.7810
LOGSTR1=	-10.0	Q(37.50)=	8491.7423
Isotope Corr.:	0.0	Q(18.75)=	3006.4654
Egy. (cm <sup>-1</sup> ) >	0.0	Q(9.375)=	1065.3896
$\mu_a$ =	2.917	A=	7756.814
$\mu_b$ =	1.465	B=	3887.882
$\mu_c$ =	1.024	C=	2836.455

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 4 (the central Carbon atom) in the atom labeling scheme adopted.