

Species Tag:	77001	Name:	C3H8O2 I 13C3
Version:	1		13C3 1,3 propanediol,
Date:	March 2010		
Contributor:	B.J. Drouin		Conformer I

Lines Listed:	11244	Q(300.0)=	76422.0338
Freq. (GHz) <	300	Q(225.0)=	53479.9622
Max. J:	30	Q(150.0)=	31501.1715
LOGSTR0=	-10.0	Q(75.00)=	11885.7256
LOGSTR1=	-10.0	Q(37.50)=	4250.6737
Isotope Corr.:	0.0	Q(18.75)=	1504.8573
Egy. (cm <sup>-1</sup> ) >	0.0	Q(9.375)=	533.2656
$\mu_a$ =	2.917	A=	7670.9366
$\mu_b$ =	1.465	B=	3839.3622
$\mu_c$ =	1.024	C=	2823.4732

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 3 in the atom labeling scheme adopted.