

Species Tag:	76012	Name:	C3H8O2 II
Version:	1		1,3 propanediol,
Date:	March 2010		v = 0,1
Contributor:	B.J. Drouin		Conformer II

Lines Listed:	21295	Q(300.0)=	90836.7418
Freq. (GHz) <	300	Q(225.0)=	53600.5819
Max. J:	30	Q(150.0)=	22443.3757
LOGSTR0=	-10.0	Q(75.00)=	3038.0698
LOGSTR1=	-10.0	Q(37.50)=	139.5607
Isotope Corr.:	0.0	Q(18.75)=	0.8145
Egy. (cm <sup>-1</sup> ) >	107.0	Q(9.375)=	0.0001
$\mu_a$ =	1.80	A=	7701.2351
$\mu_b$ =	2.13	B=	3891.2952
$\mu_c$ =	-0.65	C=	2854.5575

The data set used is from D. F. Plusquellic et al. J. Phys. Chem. A 2009, 113, 12911-12918. The dipole moment and conformer energy is from theory. The partition function was calculated with a summation over predicted energy levels up to  $J = 250$ .