

Species Tag:	63006	Name:	HNO ₃ 2ν ₉ /ν ₅
Version:	2		Nitric acid
Date:	Jul. 2004		
Contributor:	B. J. Drouin, E. A. Cohen, D. T. Petkie		
Lines Listed:	105483	Q(300.0)=	110248.049
Freq. (GHz) <	2114	Q(225.0)=	60668.605
Max. J:	150	Q(150.0)=	30214.599
LOGSTR0=	-10.0	Q(75.00)=	10483.257
LOGSTR1=	-8.0	Q(37.50)=	3709.987
Isotope Corr.:	0	Q(18.75)=	1315.069
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	467.431
2ν ₉			
μ _a =	1.80859	A=	13010.9873
μ _b =	-1.14813	B=	12099.9231
μ _c =		C=	6260.6373
ν ₅			
μ _a =	1.80859	A=	12962.656
μ _b =	-1.14813	B=	12025.872
μ _c =		C=	6242.237

The data set used in this fit is that of D.T. Petkie *et al.*, Journal of Molecular Spectroscopy 218 (2003) 127, 130, references cited therein and cm wavelength data from Perrin *et al.* Journal of Molecular Spectroscopy *in press* (2004). The analysis follows that of Petkie *et al.* in the internal axis system, the dipole moment has been adjusted from the gs PAS to account for this. There are many unresolved asymmetry multiplets in the data set. For the purpose of fitting, these were usually assigned to a single component. The merged file reflects this. The dipole moment was taken from the remeasurements report by A. P. Cox and J. M. Riveros, 1965, J. Chem. Phys. **42**, 3106. The partitioning of this molecule into accessible vibrational states is over 30% at room temperature. Since the full rotational-vibrational partitioning is well known for states < 1000 cm⁻¹, the vibrational partitioning has been included in the catalog prediction. For states below 1000 cm⁻¹, the sum-over-states calculation is explicitly used, for states above 1000 cm⁻¹, the harmonic-oscillator approximation is used. Comparison of the H.O. approximation and the sum-over-states method for states below 1000 cm⁻¹ shows agreement to <0.2% at 300 K. Truncation of the sum-over-states method to J < 99 produces less than 0.003% error. No quadrupole assignments were available for these states, however, for consistency with other HNO₃ catalog files, the ¹⁴N spin states are included in the calculation.