

H2O Vapor Parameters

pi	nu 0	e	h bar	m sub e	a0	c	mp	
3.1415927E+00	1.2566371E-06	1.6021892E-19	1.0545888E-34	9.1095345E-31	5.2917706E-11	2.9979246E+08	1.6726486E-27	
	epsilon 0	uB	eV/cm^-1		aH		md	
	8.85E-12	9.27E-24	0.000123985		5.29465E-11		3.3435860E-27	
			H2O Exp					
			2.02E-10	DeKock	aD			
			2.05E-10	Miessler	5.29321E-11			
a (m)	b (m)	c' (m)	2c' (m)	eccentricity				
2.96360E-10	2.78162E-10	1.02250E-10	2.04501E-10	0.34502				
5.60039	5.25650	1.93225	3.86450					
1								
1.5								
0.666666667								
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)			
	-15.20020	14.08285	1.35707	-0.67853	-0.43882			
Evib H2O (eV)								
0.02033								
	w (s-1)	EK (eV)						
	4.20131E+15	2.76538						
						H2O 2c'		
						0.97157		
						Exp. H2O 2c'		
	EDoppler (eV)	H2O Eocs (eV)	H2O ET (eV)	Exp. heat of vaporization (0 K eV)		0.970	Ichikawa	
	0.001444	-0.008724	0.42137	0.42137		2c' O...H (Å)		
						2.04501		
				Exp. heat of vaporization per H2O bond (0 K eV)		Exp. 2c' O...H (Å)		
				0.21069		2.02	DeKock	
						2.05	Miessler	
				Exp. heat of vaporization per H2O bond (0 K kJ/mole)		2c' O...O (Å)		
kJ/mole/eV				20.32850		3.01658		
1.03641E-02						Exp. 2c' O...O (Å)		
kcal/mole/ev				Exp. heat of vaporization per H2O bond (0 K kcal/mole)		3.02	Miessler and Ichikawa	
4.34E-02				4.86		Exp. heat of vaporization (100 °C kJ/mole)		
						40.657		
						Exp. heat of vaporization (0 K eV)		
						0.42137		
OH MO vibration	w(0) (s-1)							
u O16-H	3.3238508E+00							
0.94118	1.8213500E+00							
k(0)	1.5025008E+00	Evib(0) (eV)						
	3.08937E+13	0.02033						