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
					aD		
					5.29321E-11		
a (m)	b (m)	c' (m)	2c' (m)	eccentricity			
6.6893273E-11	4.59871E-11	4.85787E-11	9.71574E-11	0.726212391			
1.2641	0.869031344	0.918005084	1.836010167				
1							
1.5							
0.666666667							
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)		
Evib H2O (cm^-1)	-81.87146099	29.64211029	32.38330431	-16.19165216	-49.65579854		
3755.93							
Evib H2O (eV)					-49.652637		
0.465679785					match 2XH2+O		
Evib D2O (cm^-1)	w (s-1)	EK (eV)					
2787.92	6.24996E+16	41.13833376					
Evib D2O (eV)							
0.345660858							
				Emag			
				0.114411043			
		0.794402					
	EDoppler (eV)	H2O Eocs (eV)	H2O ET (eV)	H2O ED (eV)	ED (kcal/mole)	Rel. Error	
	0.630041	0.397201	50.44703872	5.105907774	117.7469427	-0.00133466	
		D2O Eocs (eV)	D2O ET (eV)	D2O ED (eV)	ED (kcal/mole)	Rel. Error	
		0.457211	50.567058	5.177547	119.3990002	0.002591677	
		0.914421					
			angle of intersection				
			-0.55433737				
kcal/mole/ev			2.15836293				
4.34E-02			123.6650866				
Do H-OH	Do D-OD	theta O	56.33491343				
117.59			0.983229723				
491.99656	5.191		0.957723873				
5.099102206			1.278983339				
		theta H2 MO	73.28034739				
ET H2O		dH2 MO	0.36367	1.92445E-11			
-45.91408221		dO AO	0.55434	2.93343E-11			
cm-1/eV							
1.24E-04							
D0 O-H							
35584							
4.411739904							
ET OH	ET OD						
-31.6282799	-31.6721						