

NH3...H2O parameters

pi	nu 0	e	h bar	m sub e	a0	c	mp	NA	
3.1415927E+00	1.2566371E-06	1.6021892E-19	1.0545888E-34	9.1095345E-31	5.2917706E-11	2.9979246E+08	1.6726486E-27	6.0221415E+23	
	epsilon 0	eV/cm^-1			aH		md		
	8.85E-12	0.000123985			5.29465E-11		3.3435860E-27		
					aD				
			2.02E-10		5.29321E-11				
a (m)	b (m)	c' (m)	2c' (m)	eccentricity		r 7	E N	N hybridization factor	
2.87519E-10	2.68015E-10	1.04093E-10	2.08186E-10	0.36204		0.93084	14.53414	0.93613	
5.43333	5.06475	1.96707	3.93414						
							E of H(a0)		
1							13.60580		
2.25									
0.71215									
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)				
	-23.60741	20.75035	2.17246	-1.08623	-1.77083				
							Geometric Parameters		
Evib NH3 (eV)									
0.021843							NH3 2c'		
							1.03677		
	w (s-1)	EK (eV)					Exp. NH3 2c'		
	4.44215E+15	2.92390					1.012		
							H2O 2c'		
							0.97157		
							Exp. H2O 2c'		
							0.970		
							2c' N...H (Å)		
							2.08186		
							Exp. 2c' N...H (Å)		
	EDoppler (eV)	NH3 Eocs (eV)	NH3 ET (eV)	NH3 per N-H ET (eV)	Cal. ECoulomb/N..H (eV)		2.02		
	0.00599	-0.00493	1.75603	0.58534	0.58534		2c' N...HO (Å)		
							3.05343		
							Exp. 2c' N...HO (Å)		
				Cal. NH3 u (bond moment)	N...H Bond Energy (eV)		2.99		
				4.89196E-30	0.30558				
							Energy Parameters		
				Cal. H2O u (bond moment)					
				5.02385E-30			Bond Energy (eV)		
							0.30558		
							Bond Energy (kJ/mole)		
							29.48		
							Exp. Bond Energy (kJ/mole)		
							29 Fessenden p. 20		
NH MO vibration	w(0) (s-1)								
u N14-H	3.6399801E+00								
0.93333	1.9207475E+00								
k(0)	1.7192326E+00	Evib(0) (eV)							
	3.31854E+13	0.02184							