pi	nu 0	e	h bar	m sub e	a0	c	mp	D/C m			
3.1415927E+00	1.2566371E-06	1.6021892E-19	1.0545888E-34	9.1095345E-31	5.2917706E-11	2.9979246E+08	1.6726486E-27	2.9979246E+29			
	epsilon 0	eV/cm^-1			aH	k	md	q/e	u (bond moment)	u (bond moment) D	1.12
	8.85E-12	0.000123985			5.29465E-11	1.3806505E-23	3.3435860E-27	0.22730	1.08554E-30	0.32544	1.25
											0.25
					aD	R of Ne initial (Eq. (10.202))					
			3.21 Å	Pollack	5.29321E-11	0.63659					
a (m)	b (m)	c' (m)	2c' (m)	eccentricity		R Ne 2p3 HO final	E coul 2p3	E of Ne 2p	Hybridization Factor	R Ne 2p3 HO final	D Ne 2p3
5.99838E-10	5.75732E-10	1.68342E-10	3.36683E-10	0.28065	N	0.56329	24.15417	21.56454	0.89279	2.98080E-11	5.96160E-11
11.33530	10.87975	3.18120	6.36239		6.0221415E+23						
0.89279											
0.89279											
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)						
	-4.40464	4.27694	0.19429	-0.09714	-0.03055						
Evib Ne-Ne (eV)											
0.00240											
cm-1/eV	w (s-1)	EK (eV)									
1.239810E-04	8.10674E+14	0.53360									
kcal/mole/eV											
4.336340E-02											
kJ/mole/eV											
0.010364101											
	EDoppler (eV)	Ne-Ne Eocs (eV)	Ne-Ne ET (eV)	Cal. ECoulomb (eV)							
	0.00004	-0.00116	0.02939	0.02939							
NeNe MO vibration	w(0) (s-1)										
u Ne-Ne	4.7718313E-01										
10.00000	2.5447815E-01										
k(0)	2.2270498E-01	Evib(0) (eV)						Exp. Heat of Vaporization (	Exp. Heat of Vaporization (kJ/mole)		
	3.64891E+12	0.00240						0.02125	2.0502		
					Energy Parameters				CRC		
					u (Cm)	density (g/cm^3)	N	U (eV)	U (kJ/mole)		
			angle of intersection with Ne		1.08554E-30	1.433	4.27659E+28	0.02368	2.285		
			62.49324044			Pollack					
			#NUM!								
		theta prime	#NUM!								
		theta Ne	#NUM!								
			#NUM!								
			#NUM!								
			#NUM!								
		theta H2 MO	#NUM!								
		dH2 MO	#NUM!	#NUM!							
		d Ne HO	#NUM!	#NUM!							
Initial Parameters 2p Shell											
	Theory		r 2p3	E 2p3							
Ne5+	157.93	21	0.56329	24.154167							
Ne4+	126.21										
Ne3+	97.12										
Ne2+	63.45										
Ne+	40.96296										
Ne	21.56454										
total	507.24										