

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		1.08
	8.85E-12	0.000123985			5.29465E-11	1.3806505E-23	3.3435860E-27	0.16298	3.37329E-30	1.01129		1.18
			0 K		aD	R of Kr initial (Eq. (10.102))			polarized u (bond moment) limit	polarized u (bond moment) limit		0.18
			3.992 Å		5.29321E-11	0.97187			3.42870E-30	1.02790		
a (m)	b (m)	c' (m)	2c' (m)	eccentricity		R of Kr 4p3 HO final	E coul 4p3	E of Kr	Hybridization Factor	R Kr 4p3 HO final	D Kr 4p3	
7.27396E-10	6.98104E-10	2.04344E-10	4.08688E-10	0.28092	N	1.05429	12.90521	13.99961	0.92183	5.57905E-11	1.11581E-10	
13.74580	13.19225	3.86154	7.72308			6.0221415E+23	R Kr 4s	IP Kr6+		R Kr 4s		
							0.85802	111.0		4.54046E-11		
						R Kr 3d	IP Kr8+			R Kr 3d		
0.92183						0.528951343	231.5			2.79909E-11		
1.08480						R Kr 3p	IP Kr18+			R Kr 3p		
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)	0.32918665	785.3			1.74198E-11		
	-3.75058	3.52342	0.13643	-0.06821	-0.15895	R Kr 3s	IP Kr24+			R Kr 3s		
						0.294497922	1155.0			1.55842E-11		
Evib Kr-Kr (eV)						R Kr 2p	IP Kr26+			R Kr 2p		
0.00091						0.125424804	2928.9			6.63719E-12		
						R Kr 2s	IP Kr32+			R Kr 2s		
cm-1/eV	w (s-1)	EK (eV)				0.113067623	3971			5.98328E-12		
1.239810E-04	5.50731E+14	0.36250				R Kr 1s	IP Kr34+			R Kr 1s		
kcal/mole/eV						0.027531668	17296.56			1.45691E-12		
4.336340E-02												
kJ/mole/eV												
0.010364101												
	EDoppler (eV)	Kr-Kr Eocs (eV)	Kr-Kr ET (eV)	Cal. ECoulomb (eV)								
	0.00019	-0.00026	0.15869	0.15869								
KrKr MO vibration	w(0) (s-1)											
u Kr-Kr	2.7629634E-01											
42.00000	1.4261159E-01											
k(0)	1.3368475E-01	Evib(0) (eV)										
	1.37948E+12	0.00091										
					Energy Parameters	0 K						
					u (Cm)	density (g/cc)	N	U (eV)		Klein p. 245		
			angle of intersection with Kr		3.37329E-30	3.094	2.22345E+28	0.11890		U (kJ/mole)		
			39.18859222							11.472		
			#NUM!									
			#NUM!									
		theta prime	#NUM!									
		theta Kr	#NUM!									
			#NUM!									
			#NUM!									
			#NUM!									
		theta H2 MO	#NUM!									
		dH2 MO	#NUM!	#NUM!								
		d Kr HO	#NUM!	#NUM!								
	Theory		Initial Parameters									
			r 4p3	E 4p3								
Kr5+	78.5	21	1.05429	12.905212								
Kr4+	64.7											
Kr3+	52.5											
Kr2+	36.950											
Kr+	24.35984											
Kr	13.99961											
total	271.00945											