Long-range dispersion interactions between excited states of K and rare-gas atoms

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Synopsis The long range dispersion coefficient between the ground state of rare gas atoms and low-lying states of K are calculated by using relativistic method, in which the spin-orbital interactions are included.

The long-range interaction potential plays an important role in the current research in the field of cold atoms[1-3]. such as **Bose-Einstein** condensation, ultra-cold collisions, and ultra-cold photo-association spectra. Precisely definition of the interaction potential between alkali metal and rare gas atoms has attracted much interest due to its signification in cold atom physics in recent years. For example, the stability and structure of Bose-Einstein condensation (BEC)[1] depend on the sign (and magnitude) of the scattering length, and the scattering length depends on the precise values of the dispersion constants. The long-range van der Waals dispersion coefficients between two atoms, is one of the more important parts of long-range potential.

In this work, the long-range interaction between low-lying states of K and the ground state of rare gas atoms are calculated in JJ coupled states, in which the spin-orbital interactions are included. The energy levels and transition arrays that contribute to the dispersion parameters are computed by using the relativistic semiempirical-core-potential method (RCICP)[4]. The rare gas oscillator strengths distributions are derived by using calculations of rare-gas polarizabilities and dispersion coefficients to tune Hartree-Fock single-particle energies and expectation values [5].

The present dispersion coefficients between the ground state of Ar and low-lying states of K are listed in Table 1 and compared with others available values [5]. The dispersion coefficients between the ground state of K and the ground state of rare gas atoms have been calculated in our previous paper [6]. The present results are in good agreement with the configuration interaction plus core polarization (CICP) results [5].

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	MT	C_6		C_8		C_{10}	
		Present	Other[7]	Present	Other[7]	Present	Other[7]
$4s_{1/2}$	1/2	299.37	299.3	22265	22280	2.1300(6)	2.132(6)
4p _{1/2}	1/2	578.59		76428		1.3286(7)	
4p _{3/2}	3/2	470.44	471.7	11232	11220	8.0594(5)	8.022(5)
	1/2	693.81		1.4340(5)		2.6173(7)	
$5s_{1/2}$	1/2	1784.6	1786	6.1844(5)	6.192(5)	2.5250(8)	2.529(8)
3d _{5/2}	5/2	707.73	712.0	-31943	-31900	-6.7078(5)	-6.713(5)
	3/2	1035.8		2.0671(5)		1.8168(7)	
	1/2	1199.9		5.4485(5)		2.1838(8)	

Table 1 The dispersion coefficient (in a.u.) between the ground state of Ar and low-lying states of K. The numbers in the round brackets denote powers of ten.

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