

	K ⁺	I ⁻	C
K ⁺	1.49,36.8,22.9	1.49,102.9,107.6	6.43,1.83×10 ⁻⁴
I ⁻	1.49,102.9,107.6	1.49,269.5,624.8	7.06,2.51×10 ⁻⁴

TABLE I. Potential parameters: For the interaction between the ionic species the three numbers specify a , B , and C_6 in the Born-Mayer potential $U(r)=Be^{-ar}-C_6/r^6$. For the interactions between the ions and the carbon atoms of the graphite, the two numbers specify σ and ϵ in the Lennard-Jones potential $U(r)=4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6]$, obtained from the graphite-inert gas potentials with ϵ scaled to allow for the different polarizabilities of K⁺ and I⁻. All values are in atomic units. The iodide and potassium polarizabilities are 44.5au and 5.3au with short-range damping parameters of ($b = 1.19, c = 2$) [11].