Excitation Transfer and Diffusion Property in a Very Weakly Excited Lithium Gas

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The aim of this study is a quantal computation of the diffusion coefficient, D, of excited lithium atoms Li(2p) in their parent gas Li(2s). The variation law of D with temperature, T, is also treated. The calculations are further extended to the determination of the excitation transfer cross section correlated with the process Li(2p) Li(2s) $\rightarrow$ Li(2s) Li(2p). To do so, we have constructed from recent RKR and/or ab initio data points the eight singlet and triplet potential energy curves through which an atom Li(2p) approaches Li(2s). In the short- and long-range regions, the data points are smoothly connected to the forms exp(-bR) and $1/R^n$ respectively. The phase shifts, obtained for each energy, E, and angular momentum, l, from the numerical integration of the radial wave equation, allows the calculation of the diffusion and excitation transfer cross sections Q_D and Q_{tr}. Our results show that the weighted cross sections vary with energy like $E^{-1/2}$, and the diffusion coefficient is found of the form D ~ AT/n, with n being the number density and A a constant. A semi-classical method shows that $Q_D \approx 2Q_{tr}$ and points out that the long-range R^{-3} forces are prominent in the diffusion of excited atoms in their parent gas.