Electronic radiative transitions in He($1s^2 2^{1,3}S$)-Ne weakly bound excimers

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The metastable states He($1s^2 2^{1,3}S$) are the champions in terms of radiative lifetimes of neutral atomic states, $\tau_1^0 = 2 \cdot 10^{-2}$ s, $\tau_3^0 = 7 \cdot 10^3$ s for the singlet and triplet states respectively. However, in numerous applications, e.g., in ionospheric and discharge plasmas, one deals with a metastable atom surrounded by buffer gas atoms. Thus, one needs to account for the influence of the interaction between atoms on radiative properties including lifetimes and spectral profiles. The issue is of topical in the case of low temperatures when processes of recombination lead to the formation of clusters and dimers containing excited atoms. This work accounts for reaction of radiative transitions in the weak bound He($2^{1,3}S$)-Ne excimers and focuses on the calculations of the averaged lifetimes and spectral profiles produced by optical transitions from vibrational states of the excimers. For large interatomic distances about $10a_0$ it had been shown [1] that the interaction with a Ne atom destroys the spherical symmetry of the He(2^1S) state via admixture of *p*-atomic states of the He atom that increases the probability of radiation in ~10^3 times.

The starting point of the present calculations for small distances about $5a_0$ is *ab initio* potential energy curves and electronic dipole transition moment [2]. The calculations have revealed the existence of shallow potential wells with four vibrational states in the He(2^1S) case and eleven vibrational state in the He(2^3S) case. Discrete Variable Representation basis functions sinc(R) for nuclear wave functions were used to calculate the positions of vibrational levels and the nuclear wave functions.

The lifetimes of weakly bound He($2^{1,3}S$)-Ne excimers as well as temperature dependences of lifetimes and spectral profiles averaged over the Boltzmann distribution have been calculated. Bound-bound transitions contribute 16% in the singlet case and 2% in the riplet case to Franck-Condon factor, the rest is coming from the bound-free transitions. Radiative transitions mainly lead to the formation of the ground-state He and Ne atoms with the kinetic energy of relative motion in the range of 0-0.03eV. The interaction at small distances results in substantial decreasing of lifetimes: $\tau_1 = 6.7 \cdot 10^{-7} \tau_1^0$ for singlet and $\tau_3 = 6 \cdot 10^{-10} \tau_3^0$ for triplet.

Although He-Ne gas mixtures and, in particular, emission of the excited Ne atoms have been intensively studied since the advent of the first gas laser it would be interesting to study transitions in the He atoms under temperatures below 100 K, when the process of the excitation transfer is negligible [3], but recombination processes should produce a large number of the excimers.

References:

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