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Systematic calculations of oscillator strengths in noble gases.

Oleg Zatsarinny and Klaus Bartschat

Drake University, Des Moines, USA

oleg_zoi@yahoo.com

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The B-spline box-based close-coupling method [1,2] was applied for extensive calculations of the transition probabilities in the noble gases Ne, Ar, Kr, and Xe for energy levels up to $n = 12$. Individually optimized, term-dependent sets of non-orthogonal one-electron radial functions were used to account for the strong term dependence in the valence orbitals. The core-valence correlation was introduced through multi-channel expansions, which include the ns^2np^5, $nsnp^6$, and $ns^2np^4(n+1)\ell$ target states. The inner-core correlation was accounted for by employing multi-configuration target states. Energy levels and oscillator strengths for transitions from the np^6 ground-state configuration as well as transitions between excited states were computed in the Breit-Pauli approximation. The present calculations provide the most systematic *ab initio* radiative data for noble gases: they include the lifetimes and oscillator strengths for 299 states and 11300 transitions in Ne, 359 states and 19000 transitions in Ar, 212 states and 6450 transitions in Kr, and 125 states and 2550 transitions in Xe. We obtained excellent agreement with existing experimental data in the case of Ne and overall very good agreement for Ar and Kr, except for a few transitions to closely spaced $(n+1)s$ and *nd* states. In Xe, very close agreement with experiment was obtained for excitation of the lowest 6*s* and 6*s*′ states. However, noticeable discrepancies for excitation of the nd states indicate the limitation of the Breit-Pauli approximation in this case. Good agreement with other calculations was obtained for transitions from the ground states, whereas significant discrepancies were found for transitions between excited states. Our results show that the B-spline method with non-orthogonal orbitals can be used for accurate calculations of oscillator strengths for states with intermediate n-values, i.e., exactly in the cases for which it is difficult to apply standard MCHF methods.

[1] O. Zatsarinny and C. Froese Fischer, J. Phys. B **35**, 4669 (2002).
[2] O. Zatsarinny and K. Bartschat, J. Phys. B **39**, 2145 (2006).