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Photoionization of the open-shell nitrogen atom confined in C_{60}[1]

T. W. GORCZYCA, Western Michigan University, S. T. MANSON, Georgia State University — Since almost all of the work on the response of confined atoms to ionizing radiation has considered closed-shell atoms [1], we have embarked on a program to investigate the response of open-shell atoms with confinement. To this end, calculations of the photoionization of each of the three states, ^{4}S, ^{2}D and ^{2}P, arising from the ground $1s^2 2s^2 2p^3$ configuration of the nitrogen atom confined in C_{60}, $N@C_{60}$, have been performed using a variation of the Belfast R-matrix code that we have modified to simulate the confinement [2], from the thresholds to a photon energy of 29 eV. For comparison, free atom calculations have also been done using the same methodology. The results show that the confinement has very significant effects on the cross sections, both in resonance regions and in the open continuum, both qualitatively and quantitatively. Low-energy confinement resonances are clearly seen. In addition, the ^{4}S cross sections (confined and free) are rather different from their ^{2}D and ^{2}P counterparts owing to the significant differences between the quartet and doublet final continuum states. [1] V. K. Dolmatov, Adv. Quantum Chem. 58, 13 (2009); [2] T. W. Gorczyca, M. F. Hasoglu, and S. T. Manson, Phys. Rev. A 86, 033403 (2012).

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