

Abstract Submitted
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**Photoionization of Endohedral Atoms Using R-matrix Methods:
Application to Xe@C₆₀** THOMAS GORCZYCA, Western Michigan University,
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SON, Georgia State University, CONNOR BALLANCE, Auburn University — It
is demonstrated that the effect of a static cage potential on the photoionization of
endohedrally-enclosed atoms can be incorporated into standard R-matrix calcula-
tions using one of two independent methods. For photoionization processes occurring
entirely within the fullerene, the outer-region solutions can be modified by the addi-
tional cage potential to yield phase-shifted Coulomb functions that are matched to
the inner-region R-matrix. Alternatively, if the cage potential is contained within
the R-matrix “box,” it can be directly incorporated into the formalism via simple
one-electron integral contributions to the Hamiltonian, yielding a modified R-matrix
itself. Both methods are applied to the photoionization of Xe@C₆₀ in the vicinity
of the giant $4d \rightarrow \epsilon f$ resonance, and are found to be in excellent agreement with
each other. Furthermore, good agreement with recent experimental results is ob-
tained, validating the present approach and demonstrating that the full power of the
many-electron, multi-channel, open-shell capabilities of the R-matrix method can be
brought to bear on the photoionization of confined-atom systems in general.

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