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K-shell Photoionization of Atomic Cl

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Synopsis Recent measurements of the photoionization of atomic Cl in the vicinity of the 1s thresholds have motivated the present R-matrix calculation which takes into account relativistic effects *via* the Breit-Pauli operator. The computer code CIV3 of Hibbert and Glass and Hibbert, which also includes relativistic effects, is used to obtain the discrete wavefunctions. These are constructed with orbitals generated from a carefully-chosen large scale configuration interaction expansion. The open-shell nature of the Cl atom translates into the existence of actually four 1s thresholds, ${}^3P^o{}_{0,1,2}$ and ${}^1P^o{}_1$. The results are analyzed with particular focus on the resonances leading up to the four thresholds, and the various effects that dominate the cross sections in this energy range are unraveled.

When energetic x-rays interact with atoms (molecules), many processes take place simultaneously and must all be taken into account. This is a complex problem of multi-electron correlations that manifest *via* various types of measurable relaxation effects, such as x-ray emission (fluorescence) and Auger decay; to replicate measurement, all these processes must be included at the same level of approximation.

Prompted by the recent high-resolution measurement [1], photoionization of Cl in the vicinity of the $1s^{-1}$ thresholds is studied using the R-matrix method [2].

The process of interest is:

$h\nu + 1s^2....3p^5 \rightarrow 1s....3p^5np$

An intermediate resonance state can either decay *via* autoionization, leading to ionization of Cl into the Cl^+ ion plus a free electron, or it can radiatively stabilize, leading to no charge change of the atom; there are participator Auger and radiative decays to the main lines, and there is the more important spectator Auger and radiative decays to the satellite lines. The decay pathways of radiative stabilization redirect some of the initial photoabsorption amplitude, giving a damped photoionization cross section relative to the photoabsorption cross section.

These effects are taken into account in our calculation. For the construction of the target wave functions of the atom, the radial orbitals are optimized on adequately chosen energy levels of states that are crucial to the collision problem, such as those of the relevant core excited states of the atomic system. Our orbital basis is augmented by the inclusion of a number of correlation functions chosen to improve the energies of the ionic thresholds and the ground state of the ionic target and account for orbital relaxation following inner shell photoionization. The photoabsorption and photoionization cross sections are calculated within the framework of the R-matrix wherein participator decay is taken into account as the wavefunctions involved in the autoionization transition matrix elements are included in the close-coupling expansion of the total wavefunction of Cl. To account for spectator Auger decay to the infinite number of continua, the R matrix is modified by using an optical potential [3], wherein the energies of the core-excited states of the target are analytically continued into the complex plane via, $E \rightarrow E - i\Gamma/2$, where Γ is the spectator Auger decay width and is computed in lowest-order perturbation theory using the code AUTOSTRUCTURE [4]. Results will be contrasted with the measurement [1] at the meeting and details of the calculation will be presented and analyzed.

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References

[1] W. Stolte *et al* 2013, Phys Rev A **88**, 053425
[2] A. Hibbert 1975, *Comput. Phys. Commun*. **9,** 141
[3] T. W. Gorczyca and F. Robicheaux 1999, Phys. Rev. A **60**, 1216
[4] N. R. Badnell 1986, J. Phys. B **19**, 3827

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