Atomic Data and Stark Broadening Parameters for Sn II and Sn III

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Synopsis Extensive multiconfiguration Dirac-Hartree-Fock (MCDHF) and relativistic configuration interaction (RCI) calculations of energies, transition rates and broadening parameters are reported for Sn II and Sn III, ions which are of importance for plasma modeling. Results are compared with other recent works.

The abundance of heavy elements provides information about theories of the origin and evolution of interstellar material, and the importance of the nuclear processes that created it (nucleosynthesis). In this context singly and doubly ionized tin (Sn II and Sn III) are highly interesting. For example, Sofia *et al* [1] analyzed data from the Hubble Space Telescope (HST), focusing on the Sn II line at 1400.5 Å ($5p\,^2P^o_{1/2} - 5d\,^2D_{3/2}$), and found gas-phase ratios of Sn/H in the interstellar medium that appeared to be supersolar. More recently, photospheric lines of tin were observed in ultraviolet spectra of HD 149499B obtained with the Far Ultraviolet Spectroscopy Explorer (FUSE) and the HST [2]. Sn II has also possible diagnostic applications in the plasmas found in fusion power plants, with the critically important Sn II transitions being at 5334 Å ($6p\,^2P^o_{1/2} - 6d\,^2D_{3/2}$), 5563 Å ($6p\,^2P^o_{3/2} - 6d\,^2D_{5/2}$), and 5591 Å ($5d\,^2D_{3/2} - 4f\,^2F^o_{7/2}$) [3, 4]. Finally, tin plasmas are candidates as light sources for the next-generation microlithography.

Accurate and extensive atomic data, measured or calculated, are the keys to eliminate the uncertainties in plasma models, and allowing the real nature of observed physical processes to be determined. Tin, especially Sn II, is theoretically very challenging due to the strong $5s5p^2 - nd\,^2D$ valence interaction that is difficult to describe except through explicit configuration interaction [4].

The authors present energies, transition rates and broadening parameters such as hyperfine structures, isotope shifts, and Stark-shifts for Sn II and Sn III from large-scale fully relativistic multiconfiguration Dirac-Hartree-Fock (MCDHF) and relativistic configuration interaction calculations (RCI). The calculations for Sn II include states belonging to the $5s^2np$ ($5 \leq n \leq 7$), $5s^24f$ odd parity configurations and the $5s^2ns$ ($n = 6, 7$), $5s^2nd$ ($n = 5, 6$), $5s5p^2$ even parity configurations. Valence and core-valence electron correlation effects are explicitly described and the largest expansions for the odd and even states contain, respectively, 1 900 000 and 1 300 000 configuration state functions (CSFs). The calculations for Sn III include states belonging to the $5sns$ ($5 \leq n \leq 8$), $5snd$ ($5 \leq n \leq 7$), $5s5g$ even parity configurations and the $5snp$, ($5 \leq n \leq 7$), $5snf$ ($n = 4, 5$), $5p5d$, $5p6s$ odd parity configurations. Again, valence and core-valence electron correlation are accounted for and the expansions reach sizes of a few hundred thousand CSFs. For both ions the mean errors in the calculated energies are of the order 1-2 per mille. Results are compared with experiment and other theory [5, 6, 7].

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