Core-polarization effects in singly ionized copper

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The Cu II spectrum is important in different fields of physics e.g. in plasma diagnostics, in laser physics or in astrophysics. It stands also as a useful test of the theoretical models because both correlation and relativistic effects are expected to be important in this ion and must be considered simultaneously in the calculations. However, transition rates in Cu^+ have been the subject of rather few theoretical and experimental works. In a recent study [1], the first and very accurate lifetime measurements for Cu II obtained using laser excitation of a fast beam have been reported. They have been compared with theoretical calculations performed using relativistic Hartree-Fock (HFR) method [2]. It has been found that the HFR theoretical method, including a substantial amount of configuration interaction, is in generally fair to good agreement with experiment. The experimental lifetimes however turn out to be systematically somewhat longer than the calculated values. More recently, an extensive calculation of f-values for outer shell transitions in Cu II, using both an LS-coupling approximation and the configuration interaction code CIV3, has been reported by Donnelly $et\ al.$ [3]. When compared with the experimental data of Pinnington $et\ al.$ [1], the theoretical lifetimes deduced from the CIV3 results are systematically larger (by about 13%) than the measurements.

The main purpose of the present work is to investigate the origin of the remaining discrepancies between these two sets of theoretical data (i.e. HFR [1] and CIV3 [3] data) and the beam-laser measurements [1]. Using the HFR approach including core-polarization and configuration interaction effects in a more detailed way, we show that these effects are responsible, to a large extent, for the discrepancies mentioned above. A new set of transition rates has been obtained leading to theoretical lifetime and transition probability values in excellent agreement (within 4%) with the experiment. An indicative calculation performed with the configuration interaction code SUPERSTRUCTURE demonstrates the importance of semi-empirical term energy corrections in producing reliable radiative data in a case like Cu II.

^[1] E. H. Pinnington, G. Rieger, J. A. Kernahan and E. Biémont, Can. J. Phys. 75 1 (1997).

^[2] R. D. Cowan, The Theory of Atomic Structure and Spectra (University of California Press, Berkeley, 1981).

^[3] D. Donnelly, A. Hibbert and K. L. Bell, *Phys. Scr.* **59** 32 (1999).