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STUDY OF SPECTRA OF HF VI

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Hafnium (Z = 72) is an element that could be employed in plasma-facing materials in Tokamaks [1,2] and is also produced in neutron-induced transmutation of tungsten (Z = 74) and its alloys that will compose the divertors in these fusion reactors [3]. As a consequence, their sputtering may generate ionic impurities of all possible charge states in the deuterium-tritium plasma. These impurities could contribute to radiation losses in controlled nuclear fusion devices. The radiative properties of these ions have therefore potential important applications in this field [4,5,6]. Many lines of Hf VI in UV range, precisely from 193 Å to 474 Å, have been calculated. As no experimental determination of radiative rates is available in the literature, a multiplaform approach has been adopted to carry out the present calculations so as to estimate the accuracy of the computed rates. From the comparisons of our three independent models based on both the HFR [7] and MCDHF [8,9] methods along with the calculations published by Ryabtsev et al. [5] that they used for line classification purpose, it was found that the uncertainties affecting the theoretical rates range from a few percent (for our HFR model) to ~40 % (for our MCDHF-RCI-A model) for the strong E1 transitions with S ≥ 1 a.u. With respect to the other lines, they can be highly inaccurate with uncertainties far more than 100 % due to strong cancellation effects and important gauge disagreements that render the rates highly model sensitive. This is essentially caused by the strong mixing affecting most of the Hf VI atomic states. Finally, we recommend our HFR rates except for the two lines at 223.172 Å and at 231.451 Å where the gA-values of Ryabtsev et al. [5] should be used instead with an uncertainty indicator Unc. equal to E (> 50 %), due to strong cancellation effects affecting the former for these two transitions. We have plotted in 3 figures the difference between the level energy calculated in our three independent models and the one determined experimentally by Ryabtsev et al [5]; also plotted in 3 figures the comparison of our transition probabilities, with respect to the calculation of Ryabtsev et al. [5], The ratio, gAHFR/gARYA, is plotted versus our HFR line strength, SHFR, both in logarithmic scale. Similar plots are displayed for our MCDHF-RCI-A and our MCDHF-RCI-B models.

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Abstract Category

Atomic & Molecular Physics

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