

Atomic structure calculations of He and Li-like Ti ions for interpreting astrophysical spectra

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Synopsis We are working on atomic structure calculations with main focus on the ions relevant to Astrophysics and upcoming fusion reactors like ITER. Main work comprises of first generating atomic data of ions by theoretical calculations by Grasp2k code and then use it for plasma diagnostic studies by identifying the relevant transitions.

Study of physical processes in astrophysical and fusion plasmas consists of detail analysis of high resolution atomic spectra obtained from such plasmas. The X-ray spectra from Ti, Cu, Ni and Fe K-shell and L-shell ions are particularly important for astrophysics as they are in wavelength range covered by telescopes on board space observatories like Chandra and XMM-Newton. To conduct the astrophysical plasma diagnostic studies of Active galactic nuclei (AGN), solar corona and other similar astronomical entities, a large number of accurate transition data both from theory and experiment are indispensable. Here we have calculated similar atomic data in use for these studies by multi-configuration Dirac-Fock (MCDF) formalism used in Grasp2K code. Calculations consists of ground and few low level excited states in He-like and Li-like Ti ions and some important transitions connecting these levels.

Table 1. Calculated Energy levels for He and Li-like Ti ions.

config.	Term	This work (cm ⁻¹)	NIST (cm ⁻¹)
Ti²⁰⁺			
1s ²	¹ S ₀	0	0
1s2s	³ S ₀	37923300	37923880
1s2p	³ P _{0,-1,-2}	38114400	38114760
		38124911	38125260
		38180261	38180620
1s2p	¹ P ₋₁	38308448	38308340
Ti¹⁹⁺			
1s ² 2s	² S _{1/2+}	0	0
1s ² 2p	² P _{1/2-,3/2-}	324401	323521
		386569	385666
1s2s2p	⁴ P _{1/2-,3/2-,5/2-}	37758694	37759000
		37774736	37774000
		37817431	NA

Our results are listed in Table 1, where we have presented our calculated level energies of He-like and

Li-like Ti. Here 1s² state is used as the ground state configuration and 1s2s, 1s2p as excited state configurations are used for He-like Ti ions, whereas for Li-like Ti ions 1s²2s is used as the ground and 1s²2p, 1s2s2p as excited states configurations. We compared our results of the level energies with those of NIST database [1]. It may here be pointed out that the NIST energy levels were extrapolated using experiments and COWAN code. As we can see, nearly all the computed values of ours are in good agreement with the NIST compilation; except at one point in Li-like system. In fact this level i.e. ⁴P_{5/2-} belonging to 1s2s2p configuration is not even listed in NIST database.

Remembering that Li-like ions of all the cosmically abundant elements like Ti, Fe, Ni and Cu etc. are actually used in astrophysical plasma diagnostic studies of active galactic nuclei or Solar corona, the presence of above noted level in our estimate turns out to be significant addition to the existing knowledge. It may here be pointed out that exclusion of an important level such as ⁴P_{5/2} will adversely affect the plasma diagnostic studies while calculating the electron temperature G(T_e) and electron number density R(n_e). Where G(T_e) is calculated as the ratio of forbidden plus inter-combination to the resonance and R(n_e) as the ratio of forbidden to the inter-combination transitions.

Considering the importance of including one additional energy level ⁴P_{5/2} in the existing NIST database, which makes it complete, we had also computed all important radiative transition rates like E1, M1 and M2 for both the ions under study and these radiative rates soon will be communicated in a reputed journal for publication.

References

- [1] T. Shirai *et al.* 2000 *J. Phys. Chem. Ref. Data Monograph No. 8*, 632 pages, Vol 29(2000)

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