Assessing The Accuracy Of Spectroscopic Atomic Data For S II Lines

P. Bogdanovich[a], R. Kisielius[a], G.J. Ferland[b], V.P. Kulkarni[c]

[a]*Institute of Theoretical Physics and Astronomy, Vilnius University, A. Goštauto 12, LT-01108 Vilnius, LITHUANIA*
[b]*Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA*
[c]*Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208, USA*

Absorption-line spectroscopy is a powerful tool used to estimate element abundances in the nearby as well as distant universe. The accuracy of the abundances thus derived is, naturally, limited by the accuracy of the atomic data assumed for the spectral lines. Unfortunately, atomic data such as oscillator strengths or transition probabilities are fairly uncertain for most elements beyond Mg. To improve this situation, we have recently started a project to improve the atomic data used for optical/UV spectral lines using state-of-the-art quantal codes, and incorporate them into the plasma simulation code Cloudy [1]. Here we demonstrate our approach by focussing on S II, an ion used to estimate metallicities for Milky Way interstellar clouds as well as distant damped Lyman-alpha (DLA) and sub-DLA absorber galaxies. We report new improved calculations of a large number of energy levels and the oscillator strengths for all S II electric dipole, magnetic dipole, electric quadrupole, and electric octupole transitions.

Our calculations are based on the configuration interaction (CI) method within a numerical Hartree-Fock framework and Breit-Pauli (BP) approach to include relativistic corrections. We implement significant additions to the multiconfiguration Hartree-Fock code used in previous calculations by adopting the transformed radial orbitals (TRO) [2] to describe radial functions of the electrons in virtually excited configurations with the principal quantum number $n > 3$. In parallel, we perform similar calculations using original quasirelativistic Hartree-Fock method (QRHF) [3] with TRO in order to assess the accuracy of generated atomic data because a very similar set of configurations is implemented in both BP and QRHF calculations.

The results of these improved atomic calculations are then incorporated into Cloudy and applied to a typical DLA, for illustrative purposes. Our calculations agree closely with those from previous works, and imply only modest changes ($\approx$0.04 dex) to the metallicity estimated from S II in past studies.

REFERENCES

1. G. J. Ferland et al., *PASP* **110**, 761 (1998).
2. P. Bogdanovich and R. Karpuškienė, *Lithuanian J. Phys.* **39**, 193 (1999).
3. P. Bogdanovich and O. Rancova, *Physica Scripta* **78**, 045301 (2008).