

Atomic data for opacity calculations

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Opacity calculation concerns a huge number of atomic data, including energy levels, oscillator strength, spectral line profile parameters, and photoionization cross sections. Theoretical methods, emphasizing on various physical effects with a variety of accuracy, have been employed to obtain the data. For atomic energy levels and the oscillator strength, one- and multi- configurational self-consistent schemes in both full relativistic and non-relativistic forms have been used to show how the detailed treatment of the physics, such as the electronic correlations and the relativistic effects, affects the finally calculated opacity. Quantum mechanical and semi-classical approaches have been used to deal with the electron impact broadening of the spectral lines. Efforts have been given to clarify the environmental (density and temperature) dependence of the influence of the detailed line profiles on the opacity. One channel and multi-channel close-coupling approaches have been applied in the calculations of the photoionization cross sections. With the channel coupling, we have shown the importance of the autoionizing effects for the transmission spectra. Density, temperature, and chemical components have direct influence on the atomic structure and atomic processes. Efforts have been given to display this kind of influence via a simplified way of average atom model. As examples, x-ray transmission spectra and the spectra-resolved opacities of Al, Fe, O, C, and Mg, which one often encounters when dealing with astrophysical problems, have been obtained independently based on the so-called detailed-term (or level)-accounting treatments for the atomic data.