Highlights of Astronomy, Vol. 13
International Astronomical Union, 2003
O. Engvold, ed.

TIPTOPbase

P. Palmeri
NASA Goddard Space Flight Center, Code 662, Greenbelt, MD 20771, USA

C. Mendoza
Centro de Física, Instituto Venezolano de Investigaciones Científicas (IVIC), PO Box 21827, Caracas 1020A, Venezuela

Abstract. An overview of the online atomic database referred to as TIPTOPbase is given, in particular its opacity server (OPserver) and current developments regarding online atomic structure calculations. Efforts to include atomic data for X-ray line modeling and to integrate TIPTOPbase within the International Virtual Observatory Alliance (IVOA) are also mentioned.

1. Introduction

TIPTOPbase is a public atomic database service for astrophysical applications that has been available on the Internet since 1993, being currently accessible from the URL `http://heasarc.gsfc.nasa.gov/topbase`. It offers the community the atomic data sets that were generated in the Opacity Project (The Opacity Project Team 1995,1996), IRON Project (Hummer et al. 1993), and more recent efforts (e.g. UKRmaX) to compute atomic data for X-ray line modeling. It lists both *LS*-coupling and fine-structure data, includes graphic processing, and is fully documented. We briefly describe below its present modules and some recent developments to improve data content and access capabilities.

2. TOPbase

TOPbase (Cunto & Mendoza 1992; Cunto et al. 1993) lists *LS* term energies, f-values, and photoionization cross sections for astrophysically abundant ions (Z = 1–20 and $Z = 26$). They have been computed under the Opacity Project (Seaton 1987, The Opacity Project Team 1995, 1996) with the R-matrix method (Burke et al. 1971, Seaton 1985, Berrington et al. 1987) using multi-configuration target representations obtained with the atomic structure codes SUPERSTRUCTURE (Eissner et al. 1974) and CIV3 (Hibbert 1975). The emphasis is both on accuracy and completeness. Physical and numerical issues have been extensively discussed in the series of papers "Atomic Data for Opacity Calculations (I–XXIII)" in the *Journal of Physics B.*

3. TIPbase

TIPbase contains the atomic data sets produced in the IRON Project (Hummer et al. 1993), namely fine-structure level energies, radiative transition probabilities, electron impact excitation collision strengths and rates (effective collision strengths), photoionization cross sections, recombination coefficients, and Auger decay rates. They have been computed using the relativistic Breit–Pauli R-matrix method (Scott & Burke 1980; Scott & Taylor 1982; Berrington et al. 1995) and atomic structure codes SUPERSTRUCTURE (Eissner et al. 1974, Nahar et al. 2003) and CIV3 (Hibbert 1975). Extensive data have been calculated for ions of the iron isonuclear sequence and for the forbidden transitions (specially the infrared transitions) of the $2p^q$ and $3p^q$ (q =1–5) ions. Methods and approximations are documented in detail in the paper series "Atomic Data from the IRON Project (I–LII)" in *Astronomy & Astrophysics* and *Astronomy & Astrophysics Supplement Series.*

4. OPserver

OPserver computes with high time efficiency online Rosseland mean opacities (RMOs) and their temperature and density derivatives for a user specified temperature–density range and chemical mixture (Seaton, M.J., unpublished). The RMO for a chemical mixture M with mass density ρ and temperature T is defined as the harmonic mean (Seaton et al. 1994)

$$\kappa_{\rm R}(\rho, T, M)^{-1} = \int \frac{1}{\kappa(u)} f_{\rm R}(u) du \tag{2}$$

where $f_{\rm R}(u)$ is the Rosseland weighting function

$$f_{\rm R}(u) = \frac{15}{4\pi^4} u^4 \exp(-u)[1 - \exp(-u)]^{-2} \tag{3}$$

with $u \equiv h\nu/kT$. The monochromatic opacities are given by

$$\kappa(u) = \sum_i N_i \{\sigma_i^{\rm abs}(u)[1 - \exp(-u)] + \sigma_i^{\rm scat}(u)\} \tag{4}$$

where N_i is the number density of the ith ion and $\sigma_i^{\rm abs}$ and $\sigma_i^{\rm scat}$ its absorption and scattering cross sections. Therefore, the computation of the RMO for an arbitrary chemical mixture involves the reading of a large volume ($\sim$ 1 Gb) of ionic cross sections from secondary memory (disk) before the harmonic mean can be calculated. Data reading from disk takes up to 90% of the computing time; typical running times on the SGI Origin-2000 at the Ohio Supercomputer Center (OSC) in Columbus, Ohio, USA, are 126 s for disk reading and 14 s for computing the actual mean. On OPserver (see Figure 1), by having all the ionic cross sections permanently pre-loaded in main memory and by parallelizing the routines that take part in the calculation of the mean, the total time required to satisfy a user request on the OSC Origin-2000 is reduced to under 2 s. A small overhead for internet data transmission must be however added, but the RMO

https://doi.org/10.1017/S1539299600016774 Published online by Cambridge University Press

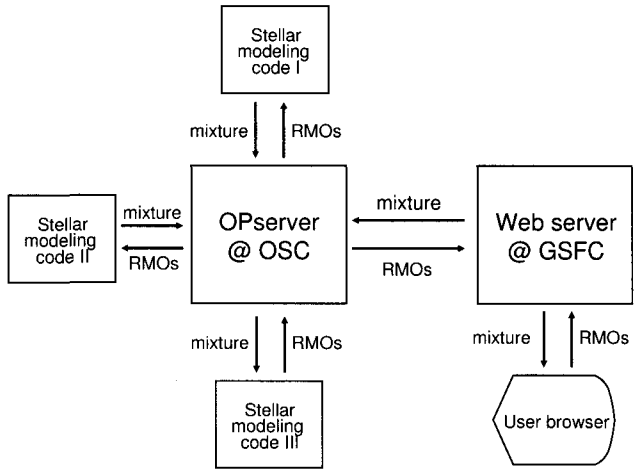

Figure 1. Online implementation of OPserver at the Ohio Supercomputer Center (OSC). User requests for Rosseland mean opacities (RMOs) for a chemical mixture can be submitted via a web page through the web server at Goddard Space Flight Center (GSFC) or from a stellar modeling code by means of linked routines.

data volume is usually small ($\sim$ 100 Kb). A user request can be performed through a web page (see Figure 1) or a stellar modeling code, say, by means of linked routines. OPserver is at present being updated with a new set of codes and monochromatic opacities that include the inner-shell contributions.

5. Online structure calculation

Since TIPTOPbase cannot always satisfy a user request for atomic data, an online implementation of the extended version of the atomic structure code SUPERSTRUCTURE (Eissner et al 1974) referred to as AUTOSTRUCTURE (Badnell 1997) is being developed that will allow the user to carry out via a web page quick calculations of acceptably accurate level energies, A-values and Auger rates for any ion. While distinct from TIPTOPbase, this service will become available in the first quarter of 2004.

6. Atomic data for X-ray line modeling

Most of the research groups that took part in the IRON Project are now involved in the computation of atomic data for X-ray applications, in particular of K and L lines in the iron isonuclear sequence. Radiative and Auger decay rates, and photoionization and electron impact excitation cross sections involving the inner shells are being studied. Lighter isonuclear sequences with $Z \leq 20$ and other systems of the iron group are also of interest. These data will progressively become available from TIPTOPbase.

https://doi.org/10.1017/S1539299600016774 Published online by Cambridge University Press

7. IVOA

As from the beginning of 2004, TIPTOPbase's home will be moved from HEASARC at Goddard Space Flight Center to the Centre de Données astronomiques de Strasbourg (CDS), France, where the possibilities of integrating it within the International Virtual Observatory Alliance (`http://www.ivoa.net`) will be considered.

Acknowledgments. Technical assistance and help in the installation and tuning of the different components of TIPTOPbase from Steve Fantasia (Laboratory for High Energy Astrophysics, Goddard Space Flight Center, Maryland, USA), Paul Buerger (Ohio Supercomputer Center, Columbus, Ohio, USA), and Francois Ochsenbein (Centre de Données astronomiques de Strasbourg, France) are gratefully acknowledged.

References

Badnell, N. R. 1997, J. Phys. B, 30, 1

Berrington, K. A., Burke, P. G., Butler, K., et al. 1987, J. Phys. B, 20, 6379

Berrington K.A., Eissner W.B., Norrington P.H., 1995, Comput. Phys. Commun. 92, 290

Burke, P. G., Hibbert, A., & Robb, W. D. 1971, J. Phys. B, 4, 153

Cunto, W., & Mendoza, C. 1992, Rev. Mex. Astron. Astrofis., 23, 107

Cunto, W., Mendoza, C., Ochsenbein, F., & Zeippen, C. J. 1993, A&A, 275, L5

Eissner, W., Jones, M., & Nussbaumer, H. 1974, Comput. Phys. Commun., 8, 270

Hibbert, A. 1975, Comput. Phys. Commun., 9, 141

Hummer, D. G., Berrington, K. A., Eissner, W., et al. 1993, A&A, 279, 298

Nahar S.N. Werner, E., Chen G.X., & Pradhan, A.K., 2003, A&A 408, 789

Scott, N. S., & Burke, P. G. 1980, J. Phys. B, 13, 4299

Scott, N. S., & Taylor, K. T. 1982, Comput. Phys. Commun., 25, 347

Seaton, M.J. 1987, J. Phys. B 20, 6363

Seaton, M. J. 1985, J. Phys. B, 18, 2111

Seaton, M. J., Yu, Y., Mihalas, D., & Pradhan, A. K. 1994, MNRAS, 266, 805

The Opacity Project Team. 1995, 1996, The Opacity Project, Vols. 1, 2 (Bristol: IOPP)