ATOMIC DATA FROM THE OPACITY PROJECT

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1. Opacity Project

The name *Opacity Project* (OP) refers to an international collaboration that was formed in 1984 to calculate the extensive atomic data required to estimate stellar envelope opacities. The project has involved research groups from France, Germany, the United Kingdom, the United States and Venezuela. The approach adopted by the OP to calculate opacities is based on a new equation-of-state formalism (see the series of papers "The equation of state for stellar envelopes", ref. [1] and contributions thereafter) and on the calculation of accurate atomic properties such as energy levels, fvalues and photoionisation cross sections (see the series of papers "Atomic Data for Opacity Calculations", ref. [2] and contributions thereafter). The theoretical framework used to compute ionic states (bound and free) and their radiative properties is based on the *close-coupling* formalism of scattering theory [3] and on the *R-matrix* numerical approach developed by Burke and collaborators [4]. Considerable improvements and extensions were introduced in the R-matrix package to adapt it for this task, thus producing a powerful computational tool to study both collisional and radiative properties of electron-ion systems. In particular, an innovative treatment of the asymptotic region has led to high efficiency and speed in computation, and allows unobserved bound states to be calculated since initial energy estimates are no longer required [5].

2. Atomic database

The systematic treatment of radiative processes by *ab initio* methods has exposed new interesting effects, e.g., PEC resonances [6]. It has also resulted in a large and useful atomic database distinguished by two key features:

(i) *Completeness* – all the astrophysically abundant ions have been considered ($Z = 1, 14$; $Z = 16$; $Z = 18$; $Z = 20$ and $Z = 26$). Non-relativistic term energies and wavefunctions for states with active electron principal quantum number $n \leq 10$ and orbital angular momentum quantum number $l \leq 3$ or 4 have been computed; of the resulting 52986 states only $\sim 20\%$ have been measured. Oscillator strengths for all the optically allowed transitions arising from such states, 1607933 in total, are listed. Photoionisation cross sections have also been calculated for all bound states that

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lie below the first ionisation threshold, choosing meshes fine enough to resolve the complicated resonance structure.

(ii) *Accuracy* – The accuracy of the R-matrix approach is comparable with the state-of-the-art in atomic calculations. Furthermore, the level of agreement with experiment is within the limits attained by such numerical methods. For instance, the theoretical wavelength accuracy is far from matching that obtained by measurements, but it is found that many theoretical radiative data, such as fvalues, lifetimes and photoionisation cross sections, can be more reliable than absolute experimental results.

Detailed auditing and comparisons with other theoretical and experimental datasets are in progress to support these assertions (see, for example, refs. [7, 8, 9]). Numerical inconsistencies or poor data lead to recalculations, and therefore the total numbers quoted above are subject to updates.

3. TOPBASE

Since the OP database is likely to be used in many research fields, we have been encouraged to enhance its accessibility by developing a portable database management system, referred to as TOPBASE, for both interactive and batch modes. A documented prototype [10] is currently being used in the OP data checking and maintenance. TOPBASE includes design considerations to facilitate work along isoelectronic and isonuclear sequences, within ionic systems and in energy or wavelength sorting. Since the program is destined to be used on different platforms and from a large variety of terminals, its on-line user interface has been implemented as a command interpreter that recognises a simple yet powerful query language. TOPBASE allows data searching in secondary storage and further data refinement and graphics in main memory to satisfy the user's ultimate requirements. Graphic capabilities are handled within the portability issue by interfacing with standard graphic packages. It is hoped to distribute both the OP data and TOPBASE as a complete package in the near future.

REFERENCES

1. Hummer D.G. and Mihalas D. (1988) *Astrophys. J.* **331**, 794. (1988).
2. Seaton M.J. (1987) *J.Phys. B* **20**, 6363.
3. Burke P.G. and Seaton M.J. (1971) *Meth. Comput. Phys.* **10**, 1.
4. Burke P.G., Hibbert A. and Robb W.D. (1971), *J. Phys. B* **4**, 153.
5. Berrington K.A., Burke P.G., Butler K., Seaton M.J., Storey P.J., Taylor K.T. and Yu Yan (1987) *J. Phys B* **20**, 6379.
6. Yu Yan and Seaton M.J. (1987) *J.Phys. B* **20**, 6409.
7. Allard N., Artru M.C., Lanz T. and Le Dourneuf M. (1990) *Astron. Astrophys. Suppl. Ser.*, **84**, 563.
8. Butler K., Mendoza C. and Zeippen C.J. (1990) in *Atomic Spectra and Oscillator Strengths for Astrophysics and Fusion Research*, J.E. Hansen (ed.), North- Holland, Amsterdam, 124.
9. Butler K. and Zeippen C.J. (1991), in *Third Atomic Data Workshop*, C.J. Zeippen and M. Le Dourneuf (eds.), *J. Physique IV*, **1**, C1-141.
10. Cunto W. and Mendoza C. (1991) *TOPBASE user's manual*, Report CSC-02-91, IBM Caracas Scientific Center, Venezuela.