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Mass production of accurate atomic data

ABSTRACT

The Opacity Project involves collaborators in France, Germany, the U.K., the U.S.A. and Venezuela. Energy levels, f-values and photoionisation cross sections are being calculated for all cosmically abundant elements, in all ionisation stages. All levels are included for which the least tightly bound electron is significantly non-hydrogenic and has a principal quantum number $n \leq 10$.

OPACITIES

Let $I(\nu, s)$ be the intensity of radiation with frequency ν , where s is a measure of distance in a direction $\hat{\mathbf{s}}$. The equation of radiative transfer is

$$\frac{dI}{ds} = -\kappa(\nu) I + j(\nu)$$

where $\kappa(\nu)$ is the monochromatic opacity and $j(\nu)$ the emissivity. If $j(\nu)=0$ and $\kappa(\nu)$ is independent of s , the solution is $I(\nu, s) = I(\nu, 0)\exp(-\kappa(\nu)s)$. Many processes contribute to κ : bound-free absorption, spectrum lines, free-free, electron scattering, *etc*. Let $\kappa(\nu, i)$ be the contribution to κ due to processes involving an initial level i. Then $\kappa(\nu, i) = N(i)\sigma(\nu, i)$ where $N(i)$ is the number-density of atoms and σ is a cross section. For bound-free transitions, σ is the photo-ionisation cross-section (multiplied by a correction factor for stimulated emission). For a spectrum line,

$$\sigma = \frac{\pi e^2}{mc} f \phi(\nu),$$

(again times a correction factor) where f is the oscillator strength and $\phi(\nu)$ the line profile normalised to

$$\int \phi(\nu) d\nu = 1.$$

For a black-body enclosure, $I(\nu) = B(\nu, T)$, the intensity of black-body radiation , and $j(\nu) = \kappa(\nu) B(\nu, T)$, which is Kirchhoff's law. For conditions in stellar interiors this law can be assumed, but $I(\nu, s)$ is not exactly equal to $B(\nu, T)$ because there is a net outward flux of radiation, $\mathbf{F}$. An approximate solution of the transfer equation gives $\mathbf{F} = -K \nabla T$ where K is proportional to $(1/\kappa_R)$ and κ_R is the Rosseland mean opacity defined by

$$\frac{1}{\kappa_R} = \left\{ \int \frac{1}{\kappa(\nu)} \dot{B}(\nu, T) d\nu \right\} \left\{ \int \dot{B}(\nu, T) d\nu \right\}^{-1}$$

with $\dot{B} = dB/dT$. This mean is an essential quantity for calculations involving the structures and evolution of the stars.

Huge amounts of atomic data are required for the calculation of κ_R . Although hydrogen and helium are the most abundant cosmic elements, at higher temperatures they are fully ionised and the dominant contribution to κ_R come from heavier elements (what the astronomers call the "metals"). Earlier studies go back to the work of Kramers and there has been a lot of more recent work, although still using atomic data which are not very accurate. Simon (1982) showed that a number of discrepancies between theory and observations of pulsating stars could be resolved by assuming that the "metal" opacities had been under-estimated by factors of about two or three, and this prompted a number of us to make new calculations using much more accurate data. The work involves collaborators in Belfast, Boulder, Caracas, Columbus, London, Munich, Nice, Paris and Urbana and we refer to it as The Opacity Project

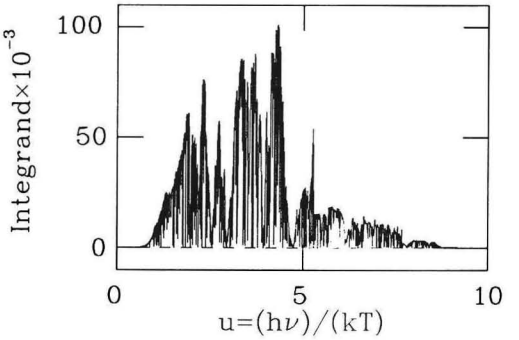

Fig. 1. The integrand for the calculation of the Rosseland mean for carbon, $\log(T) = 4.5$, $\log(\rho) = -8$. The normalisation is such that the area under the curve gives $(1/\kappa_R)$ with κ_R in atomic units per atom

MASS PRODUCTION

We require f-values and profiles for some 10^6 lines, and at least 10^5 photo-ionisation cross sections. We would not claim our data to be more accurate than the best results which have been obtained for individual transitions, using high levels of optimisation, but we do believe them to be more accurate than most of the data in the literature, and much more extensive. How can one achieve such accuracy in mass-production work ?

Our techniques (described by Berrington *et al.*, 1987) are based on those of collision theory. For atomic systems containing $(N+1)$ electrons we need to consider only

states for which not more than one electron is loosely bound, or is not bound at all (final states for photo-ionisation). We use conventional CI methods to calculate functions $\psi_i(N)$ for states containing N electrons which are all more-or-less tightly bound, and for the $(N+1)$ systems we use expansions

$$\Psi(N+1) = A\sum_i \psi_i(N)\theta_i(1) + \sum_j \Phi_j(N+1)c_j$$

where the $\theta_i(1)$ are one-electron orbitals, and A is an operator for anti-symmetrisation and vector-coupling. The functions $\Phi_j(N+1)$ are constructed using the orbitals employed in the functions $\psi_j(N)$. *An essential feature of our method is that the functions* θ_i *and coefficients* c_j *are fully optimised.* Efficiency is achieved using the Belfast R-matrix method together with a number of new features.

The orbital functions θ_i contain radial functions $F_i(r)$. A first step is to obtain non-physical functions $\Psi^{(n)}$ for an inner region $r<R$, having radial functions $F_i^{(n)}$ satisfying

$$\frac{dF_i^{(n)}}{dr} = 0 \text{ for } r = R .$$

The $F_i^{(n)}$ are expanded in terms of basis functions which satisfy the boundary condition. For each combination of angular momenta and parity only one matrix diagonalisation is required to obtain the functions $\Psi^{(n)}$. The functions Ψ for any energy E are expanded in terms of the $\Psi^{(n)}$,

$$\Psi_E = \sum_n \Psi^{(n)} C_{n,E} .$$

The Ψ_E are then matched to solutions for the outer region , $r>R$.

RESULTS FOR A SIMPLE "METAL"

Carbon, the simplest of the astronomers' "metals", has provided our first test case. Figure 1 shows the Rosseland integrand for the case of pure carbon, $\log(T) = 4.5$ and $\log(\rho) = -8$, where T is temperature in K and ρ is the density in gm cm^{-2}. Since κ_R is a weighted harmonic mean, the dips in the integrand correspond to maxima in the monochromatic opacity. There are a number of broad dips, features which had not been anticipated before the calculations were made. They are due to what Yu Yan and Seaton (1987) call *PEC resonances* (photo-excitation of the core). Their nature is illustrated in Figure 2 (from Tully, Seaton and Berrington, 1989), which shows cross sections, on logarithmic scales, for photoionisation of C III *2s5d* levels. The cross sections have series of resonances converging to the *2p* limit, and the most pronounced of these are due to processes

$$2s\,5d + h\nu \rightarrow 2p\,5d \rightarrow 2s + e$$

which give maxima at frequencies close to that for the $2s \rightarrow 2p$ transition.

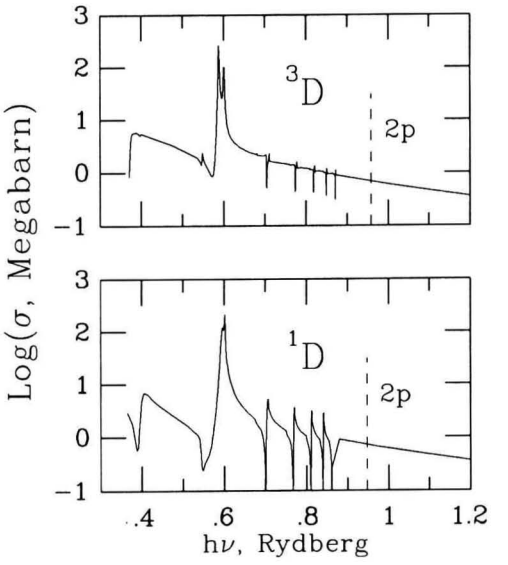

Fig. 2. Calculated photoionisation cross sections for C III *5d* levels. Note the use of logarithmic scales for σ . The features giving large maxima in the cross sections are PEC resonances (see text).

The spectrum lines also make important contributions to the mean opacity. For carbon, at temperatures and densities of interest for the stellar structure problems, our opacities are about two to three times larger than the values available at the time when Simon's paper was written. It seems likely that, when all the elements are included, we will obtain factors similar to those which he postulated.

LEVELS AND LINES

We make calculations for all cosmically abundant elements in all ionisation stages. We calculate levels for all states having an outer electron which is significantly non-hydrogenic and has a principal quantum number $n \leq 10$. Our results for energy levels may be of value for systemmatic studies of trends along iso-electronic sequences and in making identifications.

Following the notation of collision theory, we refer to the ψ_i as *target states*. For $N=1$ the targets included are $1s$, $2s$, $2p$ together with two states to allow for the polarisability of $1s$ (Fernley, Taylor and Seaton, 1987), and for $N=2$ allowance is made for the polarisability of $1s^2$ (Peach, Saraph and Seaton, 1988). For N between 3

and 10 we include all target states with configurations $1s^2 2s^x 2p^y$. For $N > 10$ the calculations become much more difficult. An example of the problems which arise is given at this meeting by H.E. Saraph and P.J. Storey who, as a part of the Opacity Project, have tackled the case of Fe VII with ground configuration $3s^2 3p^6 3d$.

I am sometimes asked whether we make much use of experimental data for the opacity work. The short answer is that we do not have experimental results for some 10^6 f-values or 10^5 photoionisation cross sections. It is, nevertheless, very important to use what experimental data are available to check the accuracy of the calculations. A recent careful compilation of all available data for f-values and lifetimes in C III, N IV and OV has been made by Allard *et al.* (1989), including all available experimental results for lifetimes. Figure 3 compares calculated lifetimes τ for 33 transitions in C III with adopted values from experimental measurements. With the exception of three "rogue" values (for which the experimental results are probably in error) the *r.m.s.* deviation is 12 per cent. Whether that gives a guide to the accuracy of the calculations or of the measurements would be hard to say: in either case the result is not too bad.

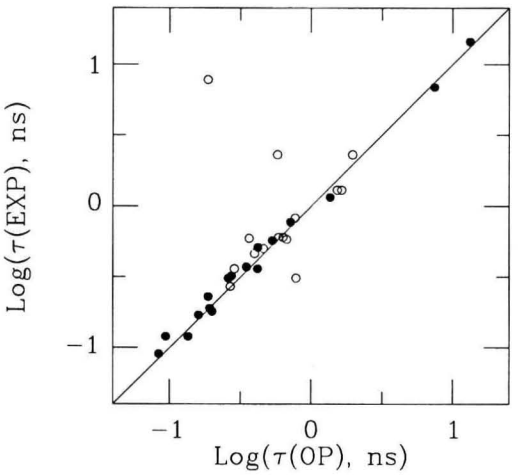

Fig. 3. Lifetimes for transitions in C III. Opacity Project results (OP) from Tully, Seaton and Berrington (1989). Experimental results (EXP) from the compilation of Allard *et al.* (1989). The filled circles are from recent measurements and cases for which several independent determinations have been made. The open circles are cases for which only one older determination is available.

PLASMA PERTURBATIONS

Stellar interiors comprise envelopes and cores. Our opacity calculations are for envelopes, the outer regions for which it is not a bad approximation to assume that atoms exist. They do not, of course, exist for states of indefinitely high excitation. In order to calculate equations of state (giving the level populations $N(i)$) it is necessary to allow for the plasma perturbations which lead to *dissolution* of the high states.

The line profiles, $\phi(\nu)$, are also determined by the perturbations of atoms by the surrounding plasma. Consider, again, the case of a transition such as $2s \rightarrow 2p$ in C IV. The profile is mainly determined by electron impacts,

$$2s + e + h\nu \rightarrow 2p + e$$

The perturbation by the added electron, which broadens the line, is similar to the perturbation which gives the PEC resonances (the only essential difference being that for the resonances the perturbing electron is initially in a bound state). The R- matrix method has been used to calculate line-profile parameters for 42 transitions in positive ions (Seaton, 1988) and the results have been used to obtain a simple approximate formula. For neutral atoms, extensive calculations have been made using semi-classical methods (Griem, 1974) and give results in good agreement with measurements (Konjevic, Dimitrijevic and Wiese, 1984). Again, we fit to a simple empirical formula (Seaton, 1989).

For systems which are hydrogenic, or nearly-hydrogenic, it is necessary to allow for the perturbations by the ion micro-field, which gives Stark shifts. Techniques have been developed for the efficient calculation of profiles in hydrogenic systems, paying particular attention to the line wings.

PUBLICATIONS

The main results from the Opacity Project are being published in two series of papers, one concerned with equations of state and the other with atomic data. More complete tabulations of numerical results will be given in a separate publication of the U.K. Institute of Physics. It is planned that all data will eventually be made available through data banks.

ACKNOWLEDGEMENTS

I thank Drs. N. Allard, M.-C. Artru, T. Lanz and M. Le Dourneuf for permission to quote from their unpublished work.

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