THE OBSERVATORY

Vol. 112       1992 FEBRUARY       No. 1106

SUMMARY OF THE RAS SPECIALIST MEETING ON

ATOMIC AND MOLECULAR DATA FOR ASTROPHYSICS

This discussion meeting, organized by K. L. Bell and P. L. Dufton, was held in the Scientific Societies' Lecture Theatre on 1991 March 8. The presentations were arranged into two sections, given either side of lunch: the first concentrated on data for atomic and ionic processes, while the second considered molecules.

The first two speakers were M. J. Seaton and K. A. Berrington who talked about the atomic data required for opacity calculations: energy levels, f-values, line profiles, photoionization, free–free transitions, and light scattering. The total amount of data required is very large (millions of lines, hundreds of thousands of photoionization cross-sections), and in most previous work use has been made of approximate atomic models which, it was hoped, would give results of a statistical accuracy adequate for the calculation of mean opacities. For the Opacity Project (which involves about 25 collaborators in 5 different countries) accurate ab initio calculations were made for all cosmically abundant elements in all ionization stages and for all non-hydrogenic levels with principal quantum numbers up to \( n = 10 \).

States for which, at most, only one electron is highly excited or is in the continuum (i.e., is a free electron, produced by photoionization) need be considered. For such states one can use methods of atomic collision theory. Consider an ion containing \((N + 1)\) electrons. One first constructs wave-functions \( \psi \) for states of \( N \) electrons which are not highly excited, using conventional methods of configuration-interaction (CI) theory; in the language of collision theory these are the 'target states'. The complete wave-function \( \psi \) for the \((N + 1)\)-electron system is then taken to be an antisymmetrized sum of products \( \psi \theta \), where \( \theta \) is a wave-function for one electron. The \( \theta \) are fully optimized using techniques based on the Belfast \( R \)-matrix codes. In all, the computer codes used for the Opacity Project atomic-data work involve some 25 000 FORTRAN statements (not including the CI codes), and have resulted in some 500 Mb of atomic data.

How good are those data? There is a dividing line at \( N = 10 \) determined, on the one hand, by the nature of the atomic-structure problem and, on the other, by the power of present-day computers. For \( N \leq 10 \) many of the data can be considered to be 'near-definitive' (f-values good to 10 per cent or better, except for cases involving delicate cancellations). It is only for a fairly small number of cases — for which highly sophisticated calculations or precise experiments have been made — that previous work gives more-accurate values.