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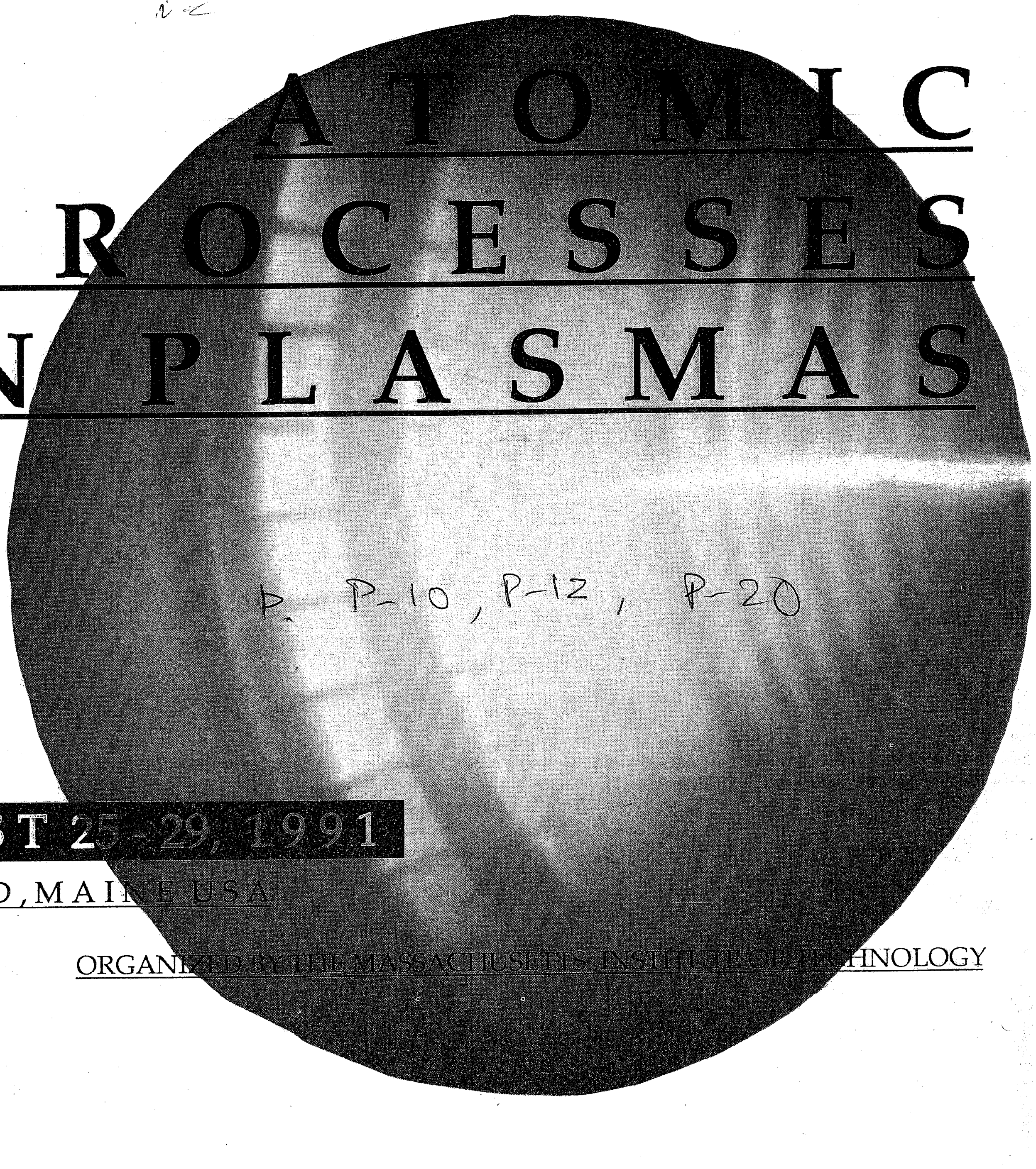

AUGUST 25-29, 1991

PORTLAND, MAINE USA

ORGANIZED BY THE MASSACHUSETTS INSTITUTE OF TECHNOLOGY

PROGRAM and ABSTRACTS

I-10

LARGE-SCALE CLOSE COUPLING CALCULATIONS FOR IRON IONS: Fe^+

By

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Extensive computations for radiative and collisional processes in heavy Iron ions are in progress. Results are presented for electron impact excitation and photoionization of Fe+ that include a large number of excited states. The R-matrix method is used for both non-relativistic and relativistic *ab initio* calculations; the relativistic effects are treated in the Breit-Pauli approximation.

It has been heretofore computationally prohibitive to employ the close coupling approximation for more than a few states of the target ion in the eigenfunction expansion. In recent years the availability of supercomputers, particularly the Cray Y-MP and the Cray-2, has enhanced the capability to enable a fairly large number of coupled channels to be included in the treatment of electron-ion systems. However the extension from small to large atomic systems is not straightforward as much greater attention needs to be given to the development of accurate eigenfunctions for the target. The final results are very sensitive to the degree of coupling between interacting channels. Consideration of the relativistic effects increases several fold the amount of computations as the number of channels with the additional fine structure in the target is much higher than in LS coupling.

Fig. 1 shows the photoionization cross section of the ground state $3d^64s(^6D)$ of Fe^+ in the close coupling approximation[1]. Further results will be presented to show that nearly a factor of two enhancement is obtained as photoionization into the $3d^6$ states of Fe^{2+} is accounted for, i.e. the photoionization of the 3d *and* the 4s electron.

Non-relativistic calculations in LS coupling including 38 states of Fe^+, and Breit-Pauli calculations for 41 fine structure states, have been carried out for electron impact collision strengths[2]. Fig. 2 shows the large enhancement affected by the presence of resonances in the forbidden transition $3d^64s(^6D) - 3d^64s(^4D)$. The earlier distorted wave results[3] are shown as dark dots. Through algebraic recoupling of the 38-state LS scattering matrices, it is possible to obtain collision strengths for 140 fine structure states, yielding excitation rate coefficients for approximately 10,000 lines in the Fe^+ spectrum.

Supported by the National Science Foundation (AST-8996215). The computational work was carried out at the Ohio Supercomputer Center in Columbus, Ohio and at the NCSA in Urbana, Illinois.

FIG 1

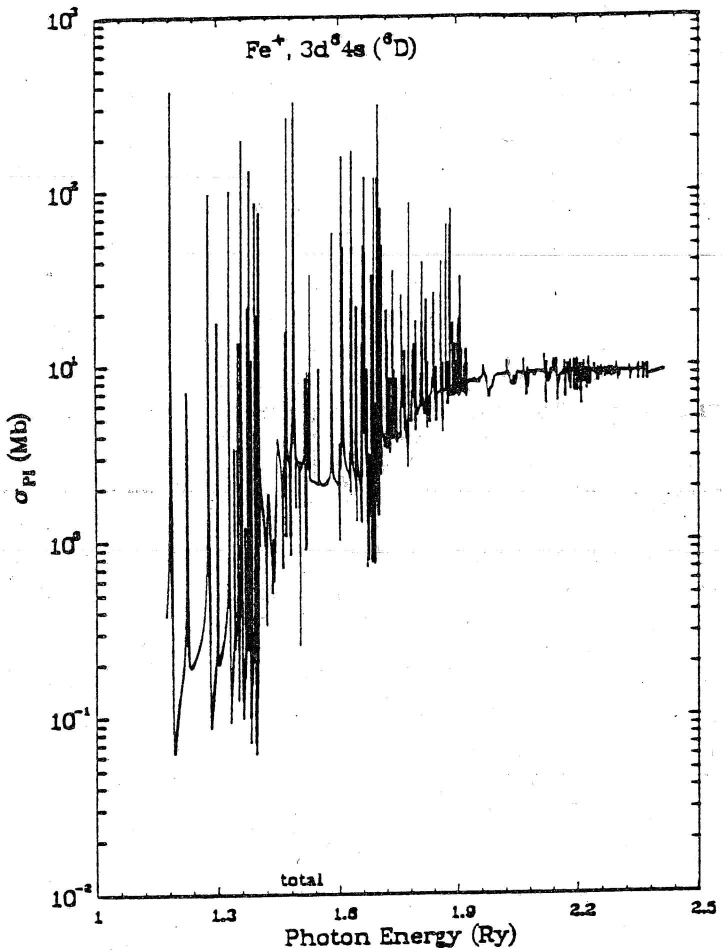
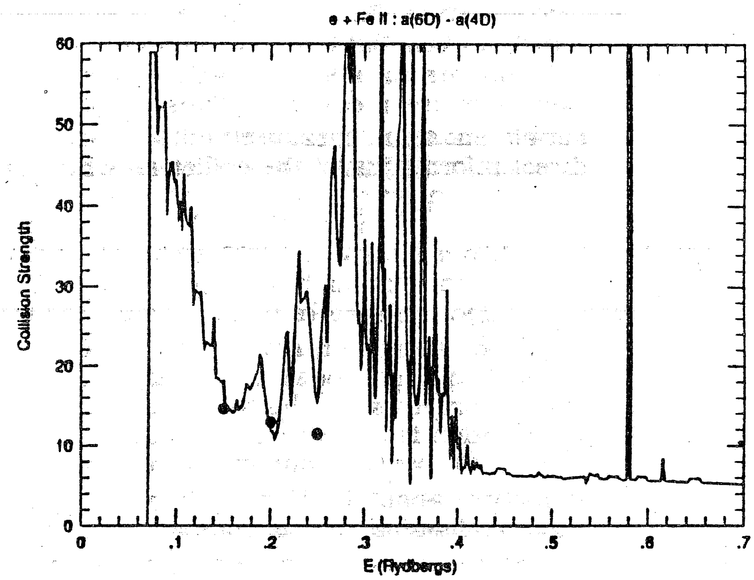


FIG. 2



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2. K.A.Berrington and Anil K. Pradhan, J.Phys.B (to be submitted).
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