

## **Evaluation of LLNL-ALICE Code Contribution**

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### **Abstract**

We summarize some of the areas of comparison with experimental data for which the ALICE code did poorly. We suggest some aspects which might be improved in the future. A crude accuracy factor is estimated as a predictive reliability based on the intercomparison exercise.

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## Introduction

Several versions of the ALICE<sup>1</sup> code were used in this code intercomparison.<sup>2</sup> Different contributors used different options in implementing the code, and the versions used by other laboratories had been modified from earlier versions of the ALICE code. Here I shall make comments on the code and input options of the LLNL contribution, and point out a few general problem areas.

The ALICE code combines the hybrid/geometry dependent hybrid precompound models, the Bohr-Wheeler fission model, and the Weisskopf-Ewing evaporation model. There are different options for level densities and fission barriers. Equilibrium gamma rays may be calculated. Reaction and inverse cross sections may be provided either by the nuclear optical model, or by a semi-classical sharp-cutoff model. Compound nucleus angular distributions are approximated as isotropic in the CM system. Precompound angular distributions may either be calculated using nucleon-nucleon scattering kinematics with or without refraction,<sup>3,4</sup> or by using the phenomenological systematics of Kalbach.<sup>5</sup> Binding energies are taken from experimental mass tables where available, otherwise from the Myers-Swiatecki mass formula.<sup>6</sup> Evaporated particles may include n,p,d and  $\alpha$ ; precompound decay involves only n and p emission, with algorithms for multiple precompound decay.

## Results and Discussion

It was seen that the many codes used in the intercomparison produced large variations in total reaction cross sections. The optical model parameter set and optical model routines used in ALICE are both in need of scrutiny and improvement. The parameters are a deduced global set,<sup>7</sup> which could better be replaced by sets more carefully chosen with respect to mass and incident energy. Additionally, for the higher energies the routine should be written relativistically. Having noted this need for improvement, I also point out that the discrepancies to be noted in these intercomparisons vis a vis experimental results, are probably outside the range of uncertainties in total reaction cross sections due to the optical model parameter sets used.

One type of problem in calculating precompound spectra may be seen in Fig. 1, where we show SDCS for (p,xn) reactions on <sup>90,91,92,94</sup>Zr for 25 MeV incident energy.<sup>8</sup> The hybrid model result from ALICE gives a smooth continuous precompound spectrum, whereas the experimental results are quite different for each of the four target isotopes, showing the effects of nuclear structure on the precompound spectra.

In Fig. 1 we show precompound calculations using single particle levels from several simple shell model oscillators to generate the few quasi-particle densities used in the precompound calculations.<sup>8</sup> In doing this we find that the resulting spectra are quite dependent on the choice of single particle levels and in turn on the assumed deformation of the excited nucleus. Thus we can improve agreement with experiment, once we know the experimental result, by a careful selection of input parameters. This may help us understand the parts of physics involved, but is of little value in making a predictive model. The question, still open, is whether or not we will one day find a set of single particle levels which, without parameter adjustment, will give a clear improvement over precompound calculations based on an equidistant spacing partial state density. Our own experience is that the single particle levels of Möller and Nix<sup>9</sup> go a long way toward this goal, but we are still very far from achieving it. I do not have a strong feeling that this goal will be achieved anytime soon.

We look next at the SDCS at incident energies of 25, 45, 80 and 160 MeV on  $^{90}\text{Zr}$  (Fig. 2) and on  $^{208}\text{Pb}$  (Fig. 3). For Zr, the (p,xn) SDCS is low by 30-40% at 45 MeV and by  $\sim 20\%$  at 80 MeV. The shapes are quite good at 25-80 MeV, but a little too hard at 160 MeV. The low cross sections cannot be explained by the reaction cross sections, and may be attributable to the equidistant partial state densities used. The discrepancy at 160 MeV is unclear. It will be interesting to see if any improvement results from a relativistic formulation, or if use of a Fermi gas (rather than equidistant) set of partial state densities would lead to any improvement. The SDCS on  $^{208}\text{Pb}$ , shown in Fig. 3, are consistent in success and failure with the results on Zr in Fig. 2.

We turn next to the DDCS - the "bottom line" in this exercise. We have not used the option of calculation based on nucleon scattering with a Fermi gas distribution of nucleons, according to the work of Goldberger.<sup>4</sup> While this option has been shown to work to a degree, the semi-empirical systematics formulas developed by Kalbach<sup>5</sup> work better. We therefore used this option. Then the two questions probed, versus ejectile energy, are how well the SDCS has calculated the mb/MeV, and how well the systematics distribute these cross sections versus angle.

At 25 MeV the DDCS do quite well to all angles (see Fig. 4). At 45 MeV incident, the results on Zr are somewhat low at all angles, reflecting the fact that the SDCS, which is the normalization of the angular distribution function, is low. The results at 80 and 160 MeV are generally satisfactory, with some suggestion that the angular distribution function gives a result slightly high at the mid-angles (up to  $60^\circ$ ), see Figs. 5 and 6.

The use of systematics gives a good DDCS spectrum at  $0^\circ$  for 160 MeV  $^{90}\text{Zr}$  (p,xn), but of course misses the very strong G-T transition (Fig. 7). Collective excitations, and excitations involving other than the simple two body N-N operator, need to be treated by a separate code or routine treating the appropriate physics. The (p,xp) DDCS are predicted as well as the (p,xn) results except that there are probably collective excitations in the last 5 MeV of the spectra which are not reproduced in the precompound routine.

## Conclusions

The ALICE code has considerable room for improvement. First, the global set of optical model parameters should be replaced using local sets optimized both for target mass and projectile energy. The work of some of the data subgroups on parameter sets will be a great help in this. Secondly, the precompound routine needs to be re-written using relativistic phase space factors. Routines need to be added to treat precompound cluster emission when the physics for this becomes clear. As the precompound calculations are extended to higher excitations, use of an equidistant spacing model in calculation of partial state densities should be checked, and use of Fermi gas spacing should be tried. Additionally, expressions for exciton densities following the first term, calculated in consideration of inconsistencies pointed out by Bisplinghoff, should be tried.

As a means of assessing predictive power of codes, it might be helpful to have plots of ratio of calculated to experimental SDCS and DDCS. This conversion would probably be a fairly major undertaking. To test the evaporation regions of these codes, we need both n and p exit channel data extending to appropriately low energies. At present, we would estimate the predictive power of the ALICE code to be within 20-30% at best for SDCS, often poorer. The results are probably good to within a factor of two for DDCS, and the limit of incident energies is around 200 MeV. This limit could be extended with extension to relativistic phase space and true Fermi gas partial state densities, but restrictions to two precompound emissions would have to be relaxed to go much beyond 200 MeV correctly, and pion physics would need to be incorporated above 260 MeV.

## References

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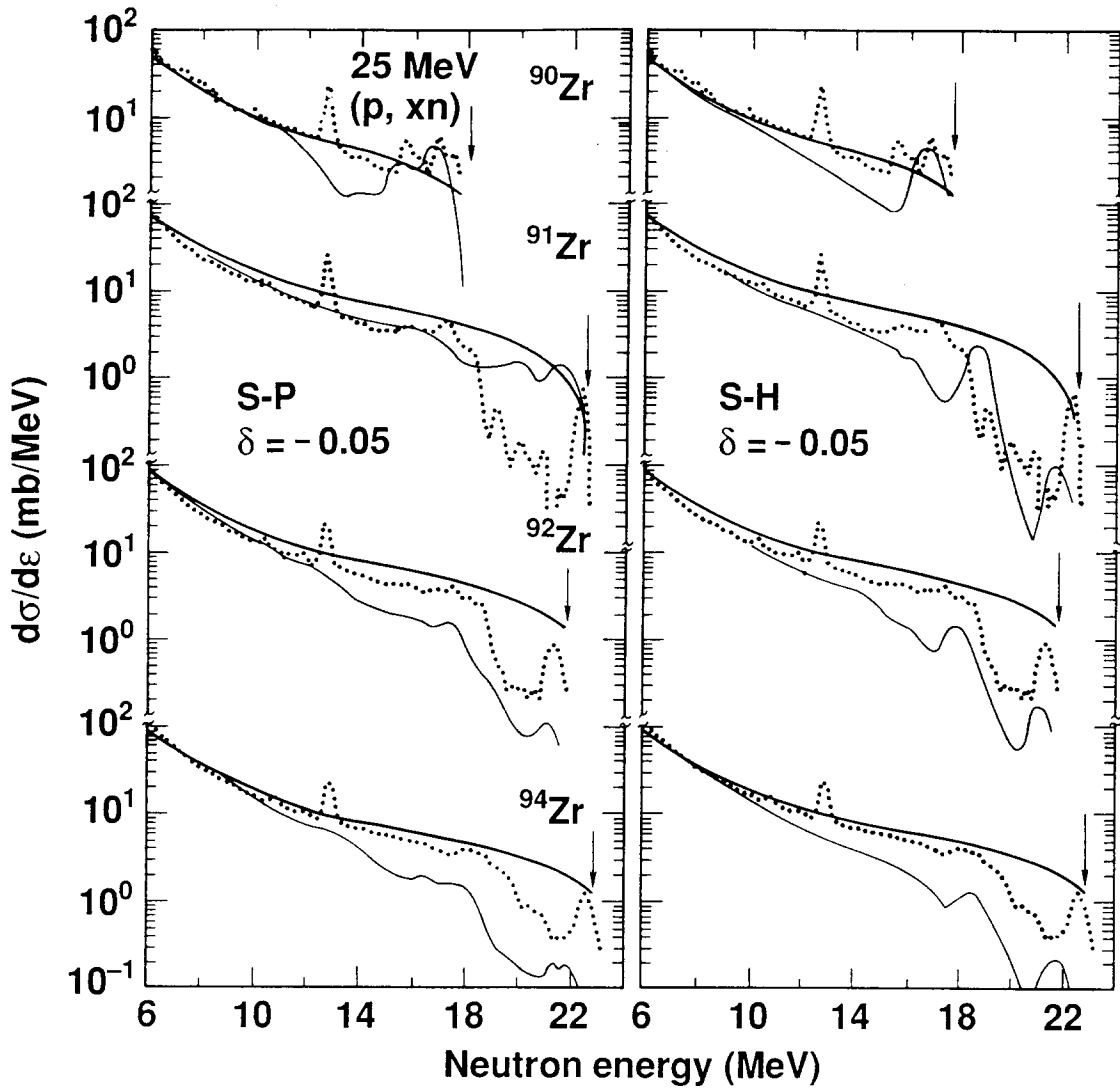


Fig. 1 Experimental SDCS for  $^{90,91,92,94}\text{Zr}$  (p,xn) at 25 MeV incident proton energy from Ref. (8), dotted line. The heavy solid line is the hybrid model result. Thin solid lines represent hybrid model results using partial state densities due to Seeger-Perisho (S-P) or Seeger-Howard (S-H) with a deformation parameter of  $\delta = -0.05$ . See Ref. (8) for details.

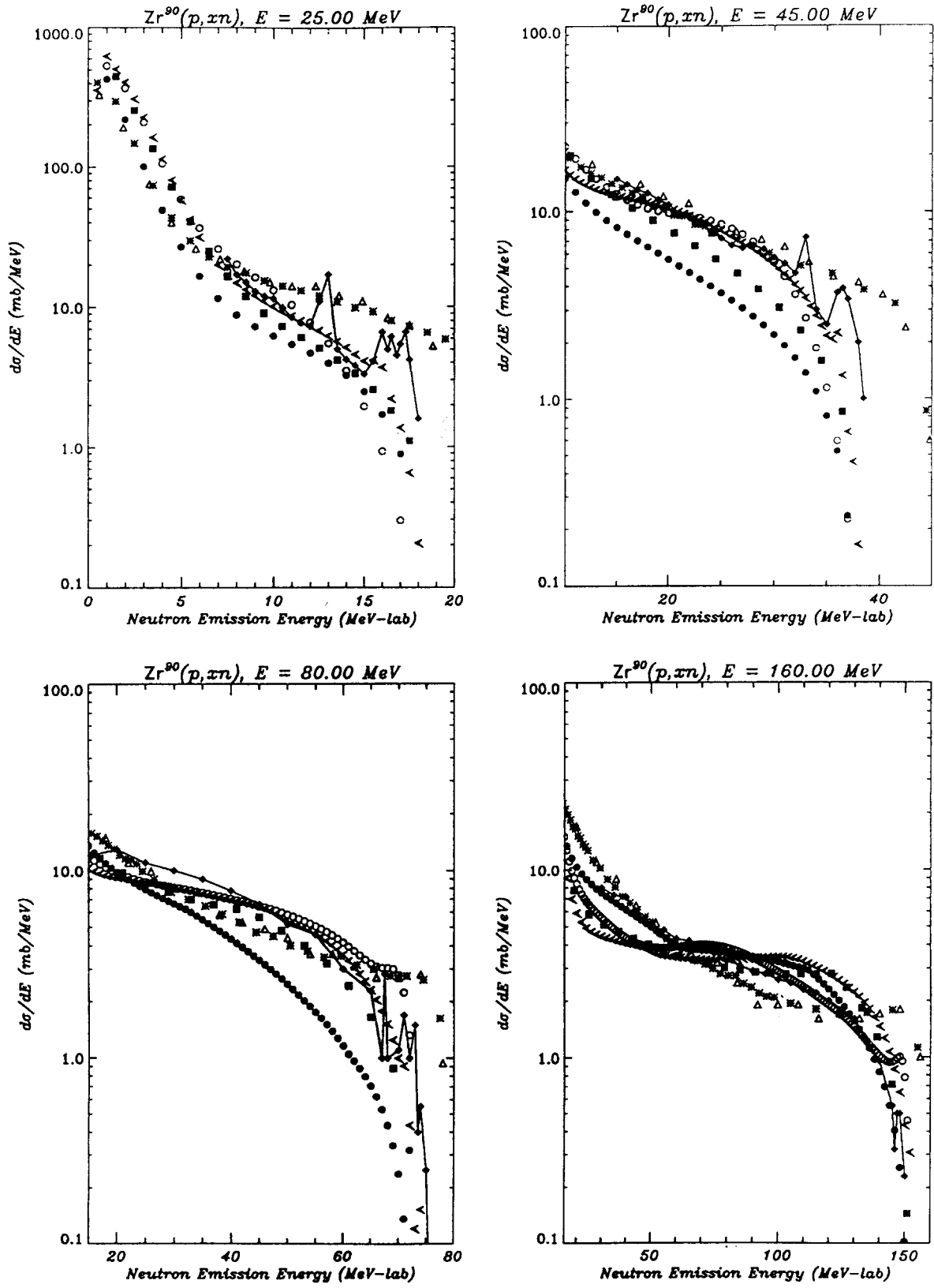
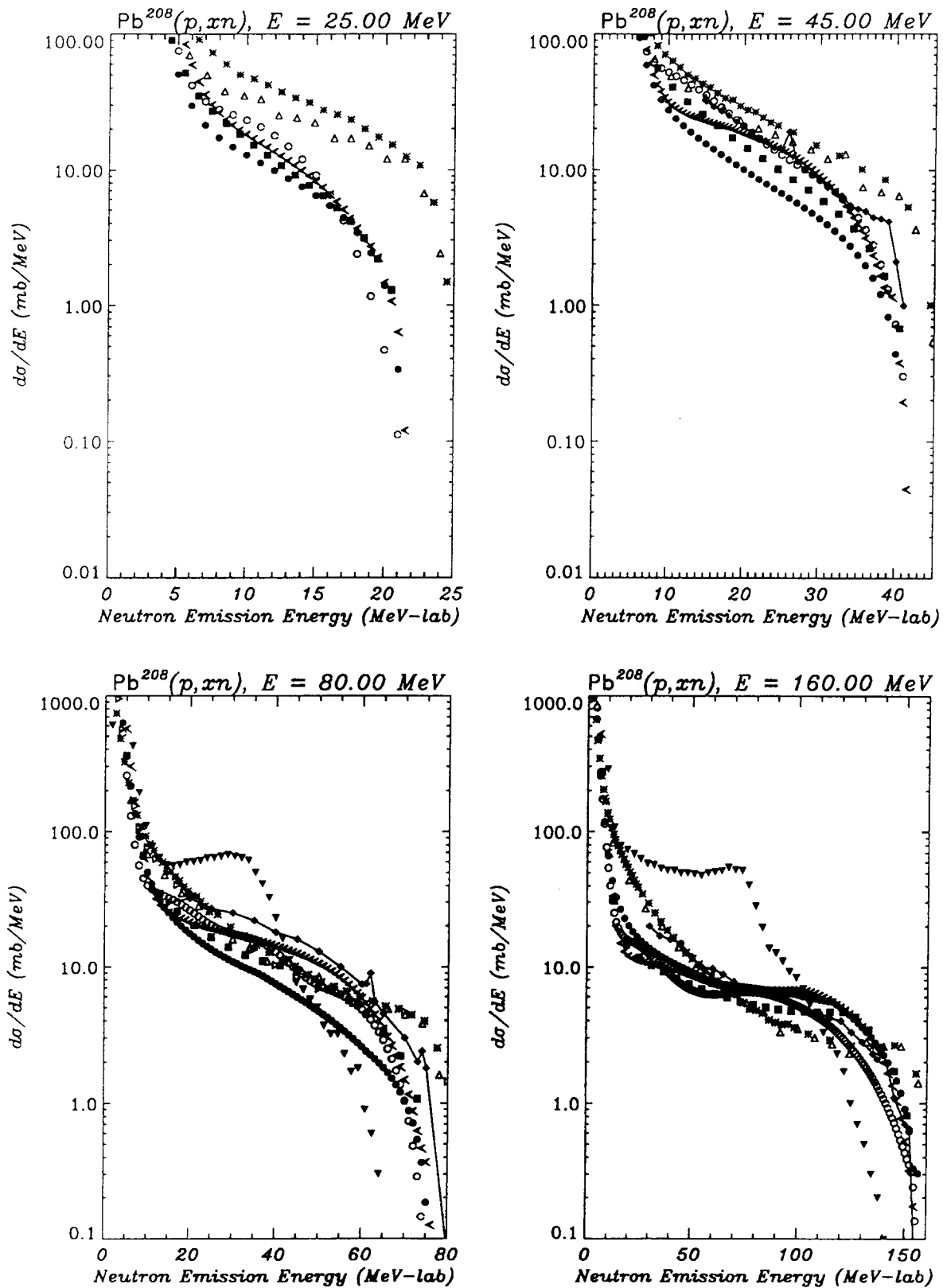


Fig. 2 SDCS for  $^{90}\text{Zr}(p, xn)$  from (2). Experimental results are joined by a solid line. ALICE results are given by solid squares. See (2) for definition of other symbols.



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Fig. 3 As in Fig. 2 for  $^{208}\text{Pb}(p, xn)$ .

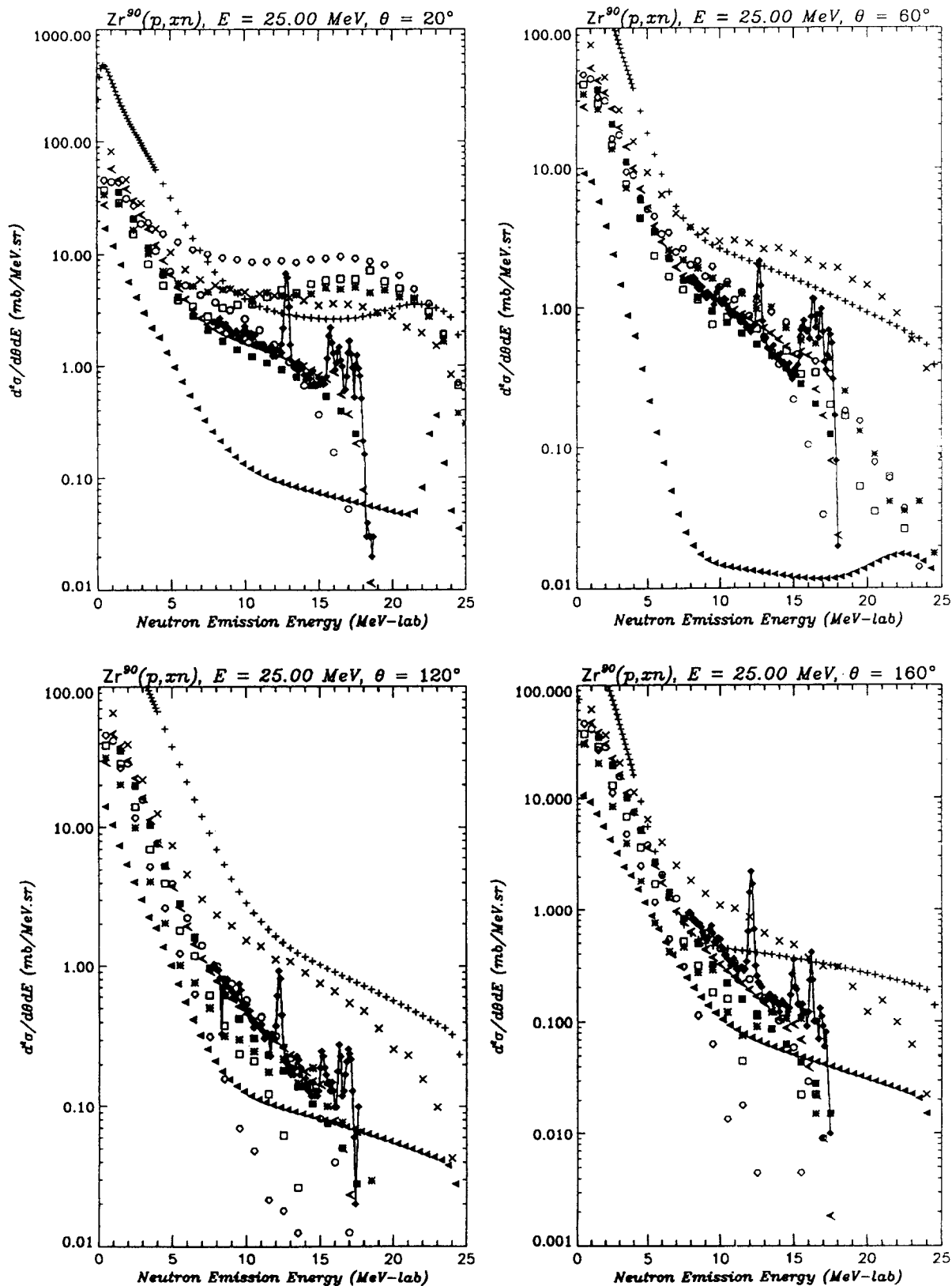


Fig. 4 DDCS for  $^{90}\text{Zr}(p,xn)$  at 20, 60, 120 and 160° for 25 MeV incident proton energies. Solid lines connect experimental data points. ALICE results are given by closed squares. This figure is from (2).



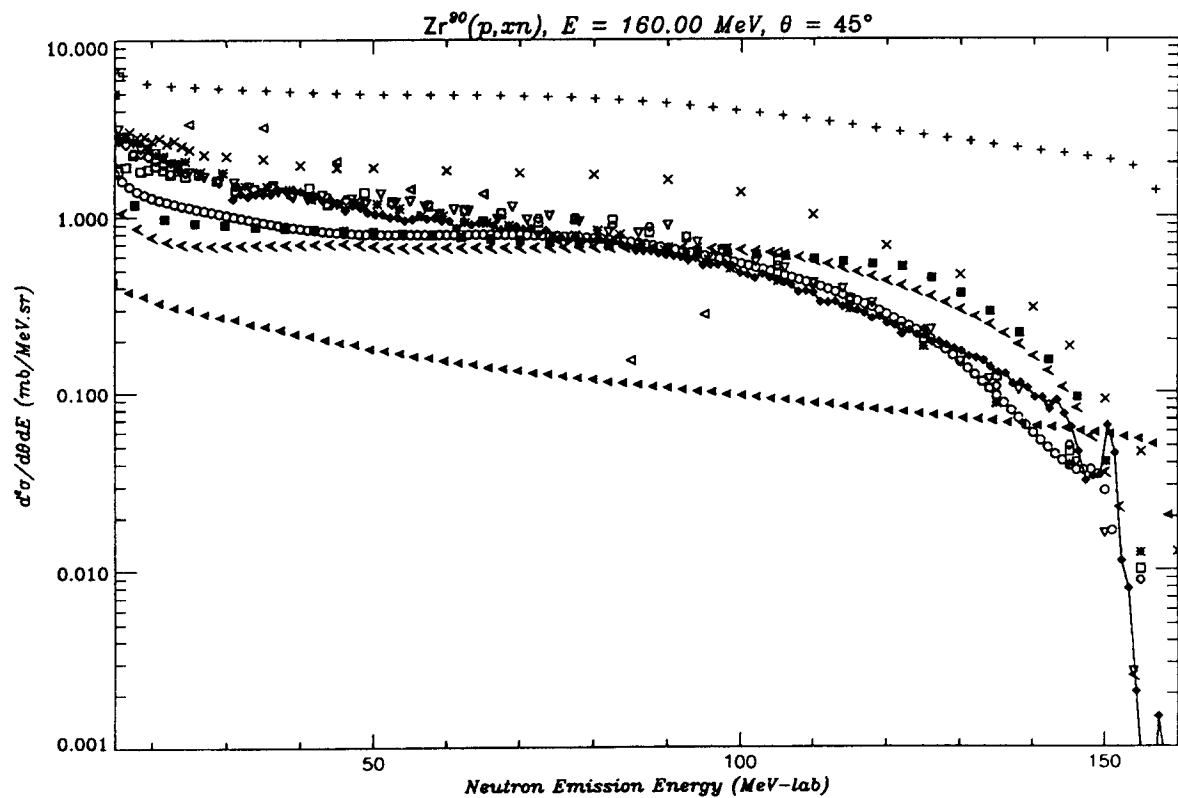
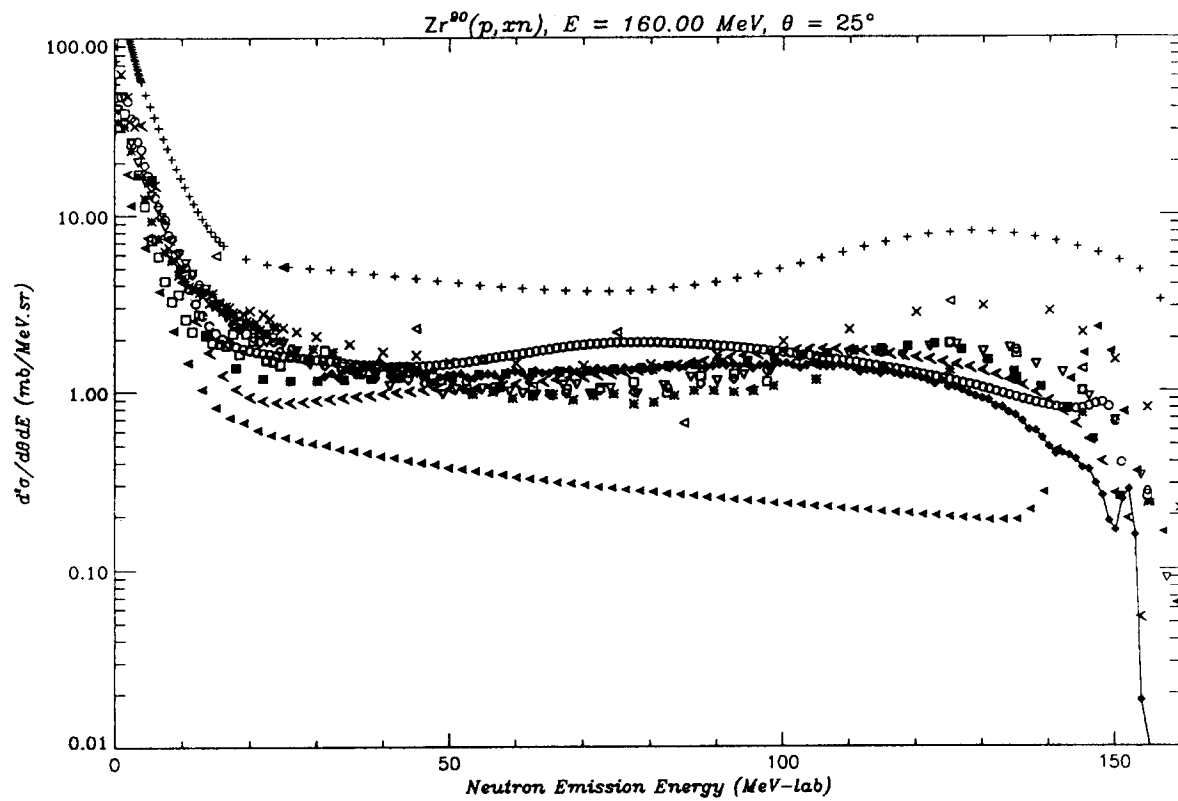


Fig. 5 As in Fig. 4 for  $^{90}\text{Zr}(p, xn)$  at  $25^\circ$  and  $45^\circ$  for 160 MeV incident protons. This figure is from (2).

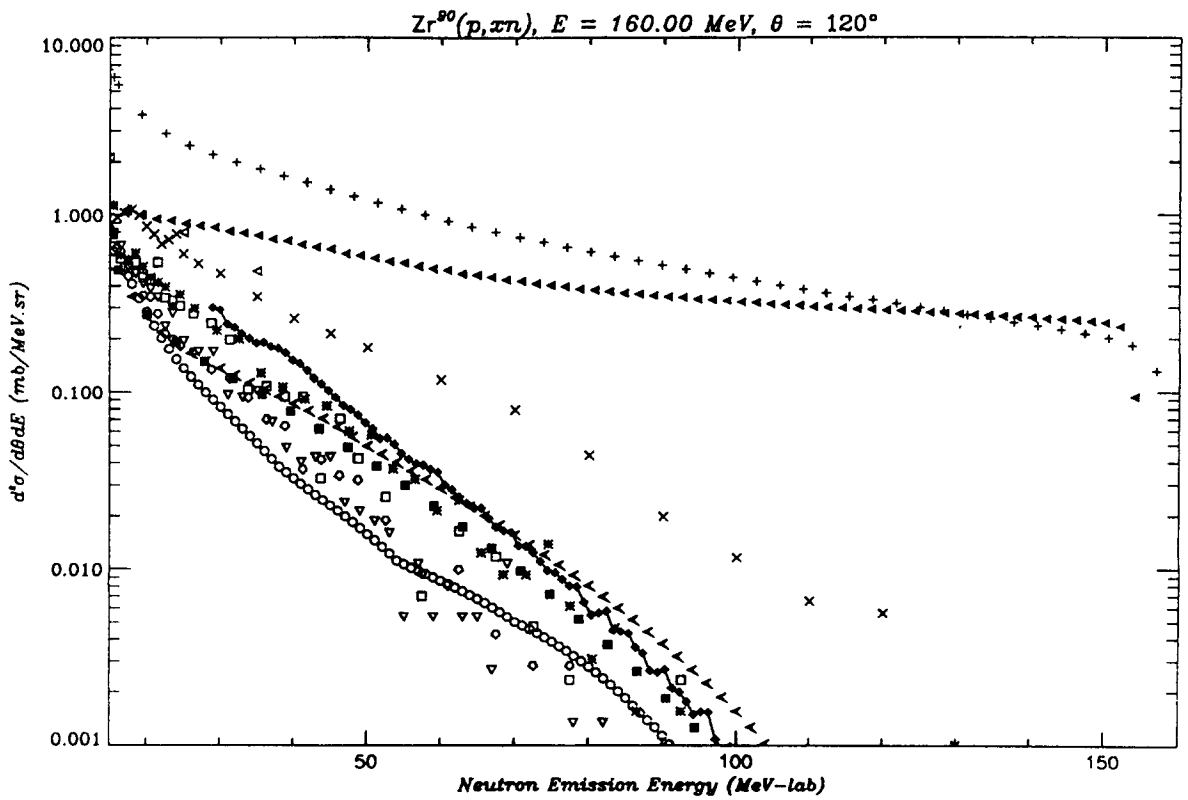
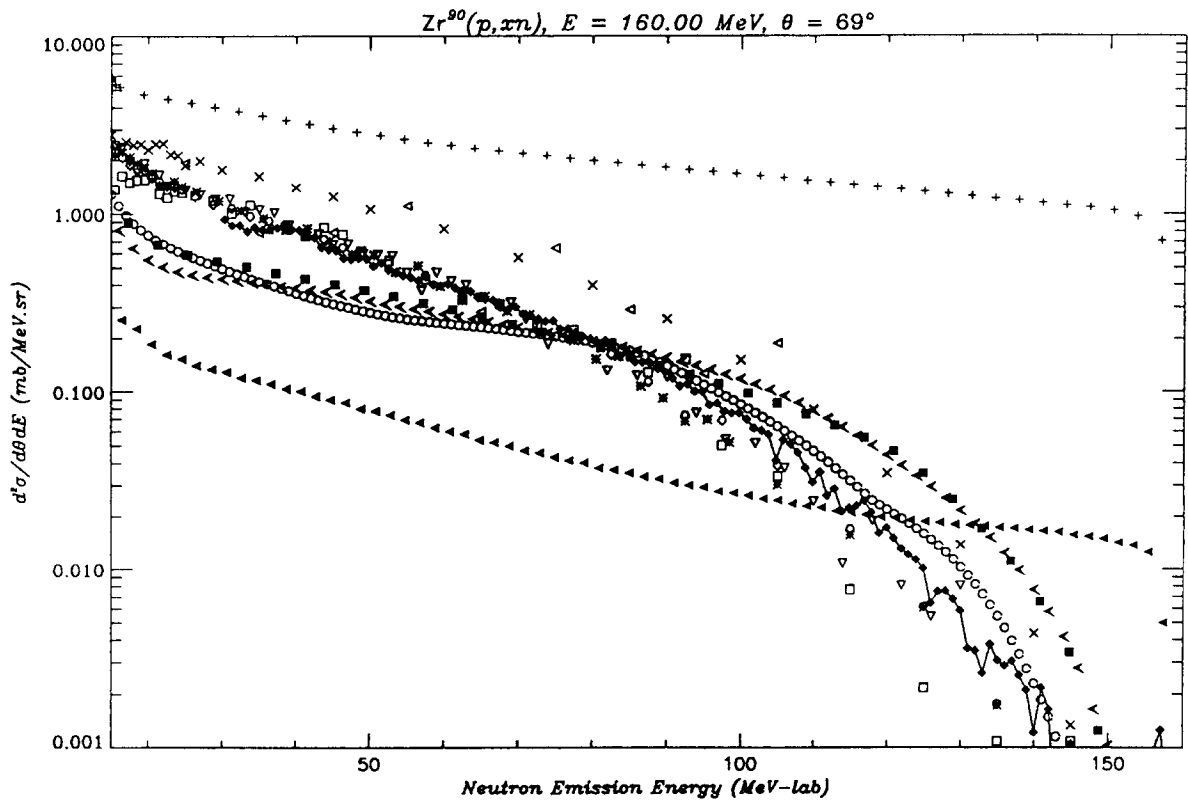


Fig. 6 As in Fig. 4 for  $^{90}\text{Zr}(p, xn)$  at  $69^\circ$  and  $120^\circ$ . Taken from (2).

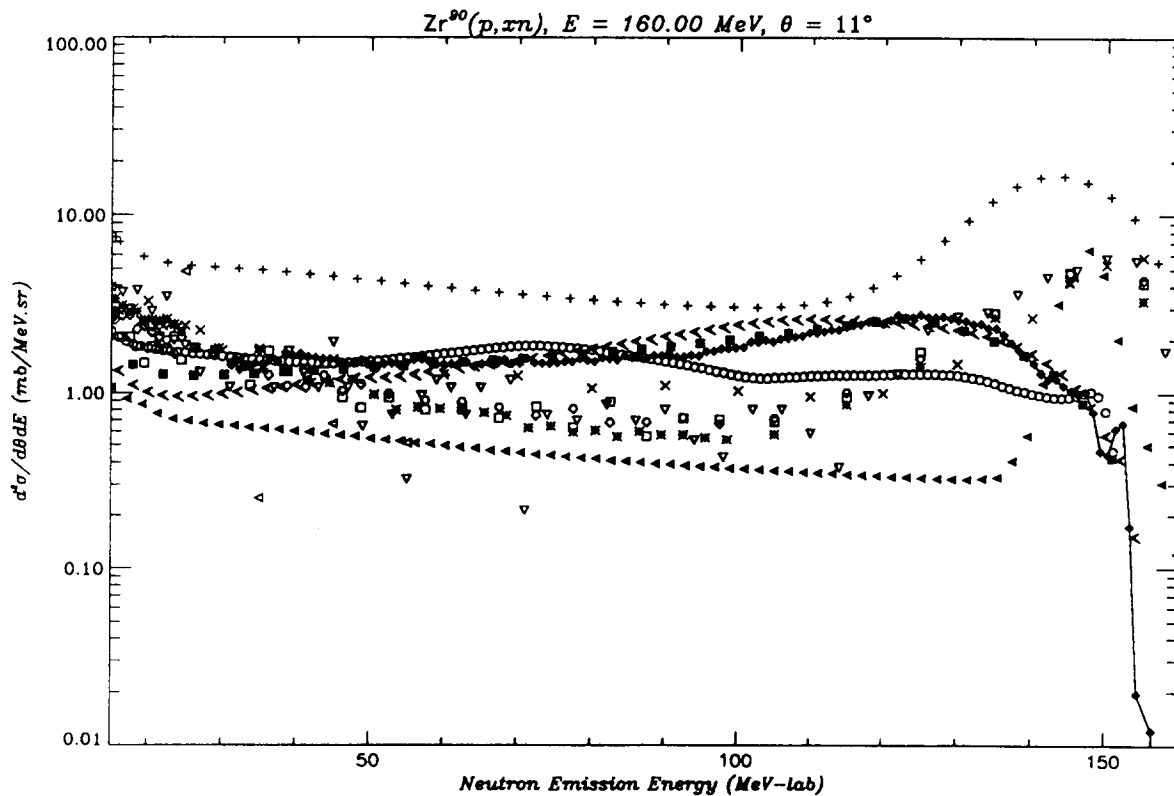
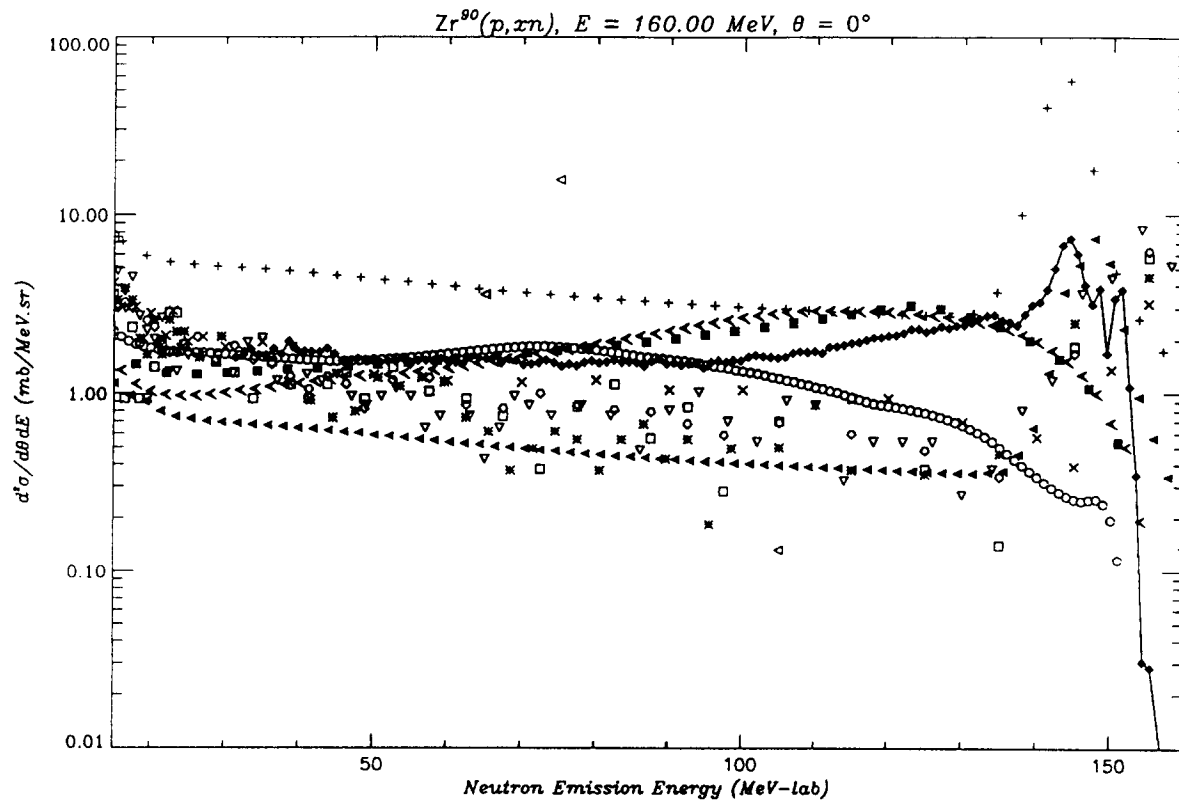


Fig. 7 As in Fig. 4 for  $^{90}\text{Zr}(p, xn)$  at  $0^\circ$  and  $11^\circ$ . Taken from (2).

