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Title:

MODELS AND CODES FOR SPALLATION NEUTRON SOURCES

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Models and Codes for Spallation Neutron Sources
Special Session within the SARE-5/SATIF-5 Meeting

SARE-5/SATIF-5 International Workshops

July **17-21, 2000,** OECD **Headquarters, Paris, France**

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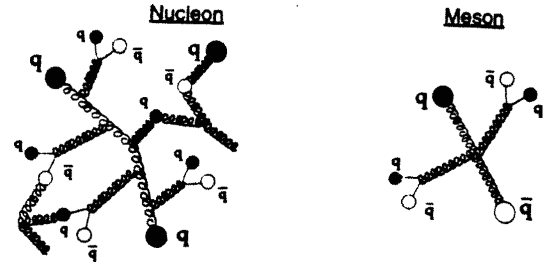
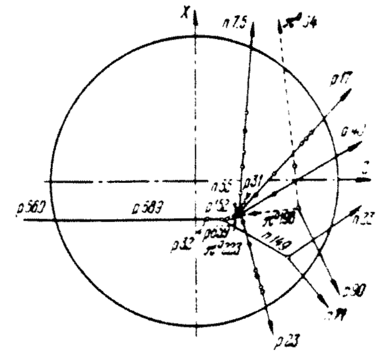
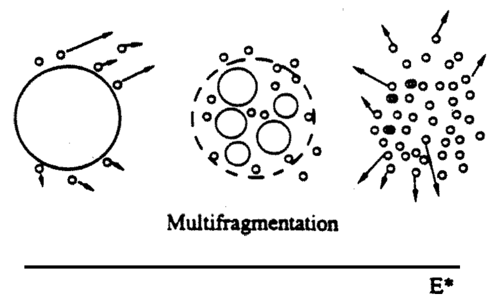
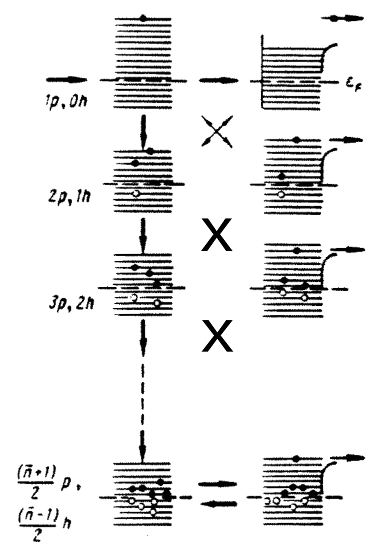
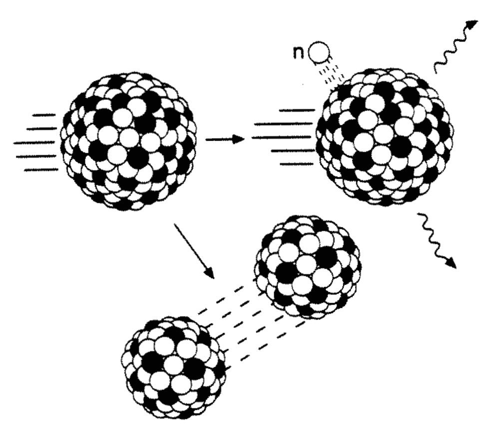
Models and Codes for intermediate Energy Nuclear Reactions

- Overview
- Evaporation
- Fission Models
- Pre-equilibrium Models
- Intranuclear Cascade
- Multifragmentation, Fermi Breakup
- Semiempirical Systematics
- High-Energy Transport Codes
- Further Work

	T_0 (MeV)	
Quark and gluon degrees of freedom: QCD Dual Parton Pomerons String Gas ... VENUS GEANT4 FRITIOF MARS FLUKA ...	10,000	 
Fast direct processes: Coupled Channels Vlasov Equation Boltzman Equation Classical Mechanic ... BUU QMD RQMD INC (Beritini, ISABEL, Dubna, ...) ...	1,000	
Pre-compound stage: FKK, TUL, and NWY Theories MSD and MSC Hybrid models Exciton models ... GNASH ALICE MPM (PREEQ1) MEM (MODEX → PRECOF) ...	100	
Compound nuclei Evaporation/Fission: Weisskopf-Ewing Theory Hauser-Feshbach Theory Statistical models of fission Dynamical models of fission ... Dostrovsky model Dresner model RAL model ORNL model ...	10	

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Multifragmentation

- Probabilistic models
- Macroscopic statistical models
- Microscopic dynamical models
- Molecular Dynamics; Quantum Molecular Dynamics
- Kinetic models
- Sequential evaporation or very asymmetric fission
- Hybrid models
- ...

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Ultrarelativistic energies

Gribov-Regge theory (Perturbative QCD doesn't apply yet)

- Quark Gluon String Model (QGSM)
- String Gas Model (SGM)
- Dual Parton Model (DPM)
- QCD Parton Model (PCM)
- Relativistic Quantum Molecular Dynamics (RQMD)
- HERWIG, ISAJET, PYTHIA, VECBOS, PAPAGENO,..., event generators
- CALOR89 code
- Lund FRITIOF code
- VENUS (Very Energetic Nuclear Scattering) code
- GEANT4 code
- MARS code
- FLUKA (FLUctuating KAscade code)
- ...

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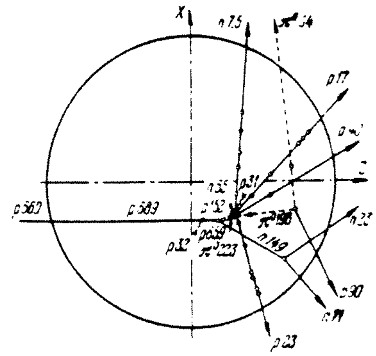
CASCADE

$$f^{cas}(\vec r,\vec p,t) = N_0\delta(\vec p-\vec p_0)exp\left[-\int_0^t dt'\rho^T < \sigma v_{rel} >\right]+$$

$$+\int_0^t dt''\rho^T\rho^{cas}\left(\vec r-\frac{\vec p}{m}(t-t''),t''\right)Q\left(\vec r-\frac{\vec p}{m}(t-t''),\vec p,t''\right)exp\left[-\int_{t''}^t dt'\rho^T < \sigma v_{rel} >\right]$$

$$Q(r,p,t)=\iint d\vec p_l d\Omega v_{rel}\frac{d\sigma(v_{rel})}{d\Omega}f^T(\vec r,\vec p_i)f^{cas}(\vec r,\vec p_j,t)\ ; \qquad j\equiv n,p,\pi^+,\pi^0,\pi^-$$



V. S. Barashenkov et al.
Sov. Phys.-Usp., Vol. 16, No. 1, July-August 1973

$\boxed{\mathcal{P}=0.3}$ $\Downarrow$ $A,\ Z,\ E,\ n=p+h,\ \vec P,\ \vec L$

PREEQUILIBRIUM

$$\frac{\partial P(E,n,t)}{\partial t}=\lambda_+(n-2,E)P(E,n-2,t)+\lambda_0(n,E)P(E,n,t)+$$

$$+\lambda_-(n+2,E)P(E,n+2,t)+$$

$$+\sum_j\int dT\int dE'\lambda_c^j(n,E,T)P(E',n+n_j,t)\delta(E'-E-B_j-T)-$$

$$-\left[\lambda_+(n,E)+\lambda_0(n,E)+\lambda_-(n,E)+\sum_j\Gamma_j(n,E)\right]P(E,n,t)$$

$$\lambda_{\Delta n}(n,E)=\frac{2\pi}{\hbar}|M_{\Delta n}|^2\omega_{\Delta n}(n,E)\ ; \qquad |M|^2\sim\frac{<\sigma(v_{rel})v_{rel}>}{V_{int}}$$

$$\Gamma_j(n,E)\sim\int\frac{\omega(n-n_j,E-B_j-T)}{\omega(n,E)}TdT\ ; \qquad j\equiv n,p,d,t,^3He,\alpha$$

Modified Exciton Model
K. K. Gudima, et al.,
Yad. Fiz., **21, 260** (1975);
S. G. Mashnik, V. D. Toneev.
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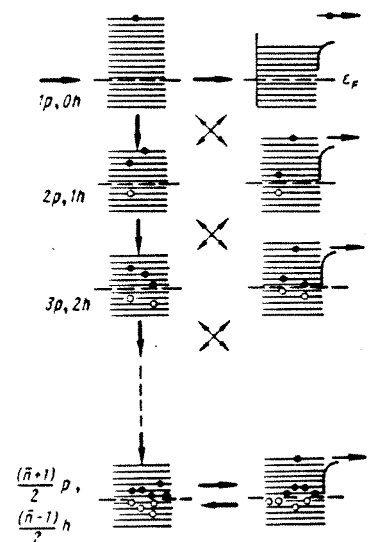


$\boxed{n=\bar n}$ $\Downarrow$ $A,Z,E,\vec P,\vec L$

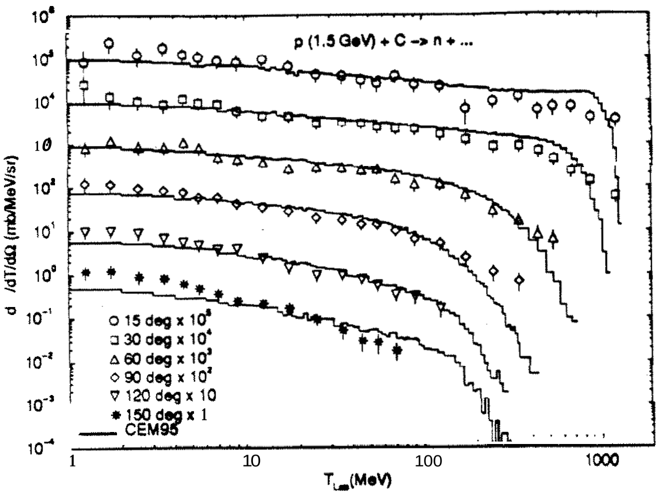
EQUILIBRIUM (COMPOUND)

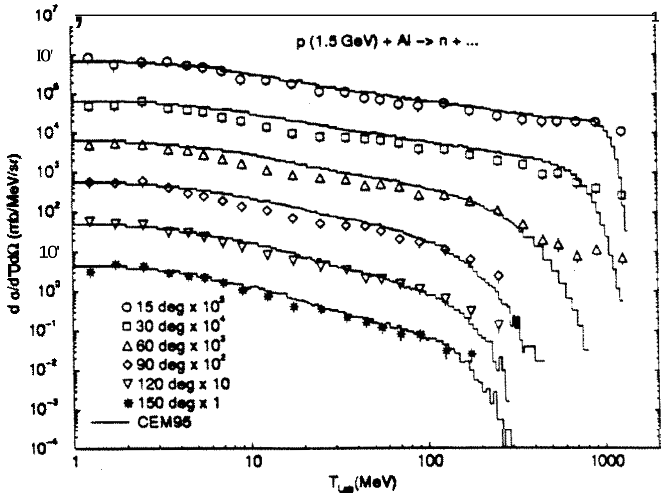
$$\omega(E)=\sum_n\omega(n,E)\sim exp2\sqrt{aE}$$

$$a=a(Z,N,E)\sim A/10\ ; \qquad j\equiv n,p,d,t,^3He,\alpha\ ;\ (+\ \text{fission})$$

Evaporation: Weisskopf-Ewing
Fission: Bohr-Wheeler
(further development,
many options)

$$\sigma(\vec p)d\vec p=\sigma_{in}[N^{cas}(\vec p)+N^{prq}(\vec p)+N^{eq}(\vec p)]d\vec p$$


p (1.5 GeV) + C -> n + ...
d /dT/dΩ (mb/MeV/sr)
T_{Lab}(MeV)
○ 15 deg x 10^5
□ 30 deg x 10^4
△ 60 deg x 10^3
◇ 90 deg x 10^2
▽ 120 deg x 10
* 150 deg x 1
CEM95


p (1.5 GeV) + Al -> n + ...
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T_{Lab}(MeV)
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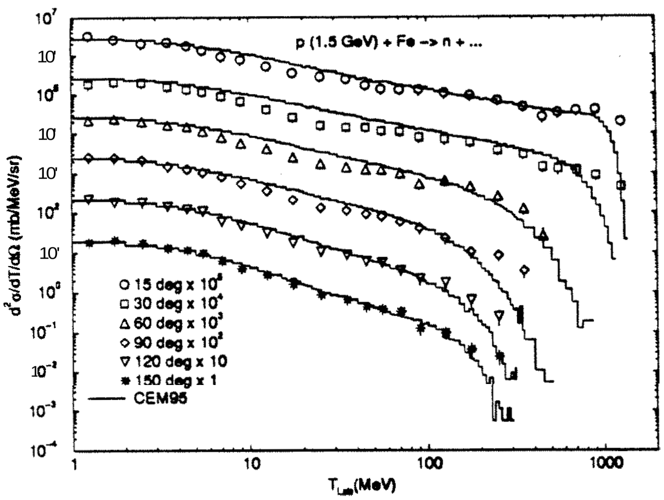
p (1.5 GeV) + Fe -> n + ...
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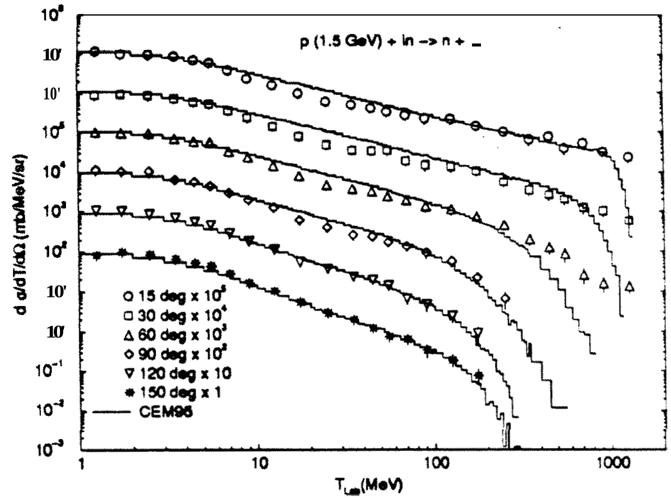
p (1.5 GeV) + In -> n + ...
d σ/dT/dΩ (mb/MeV/sr)
T_{Lab}(MeV)
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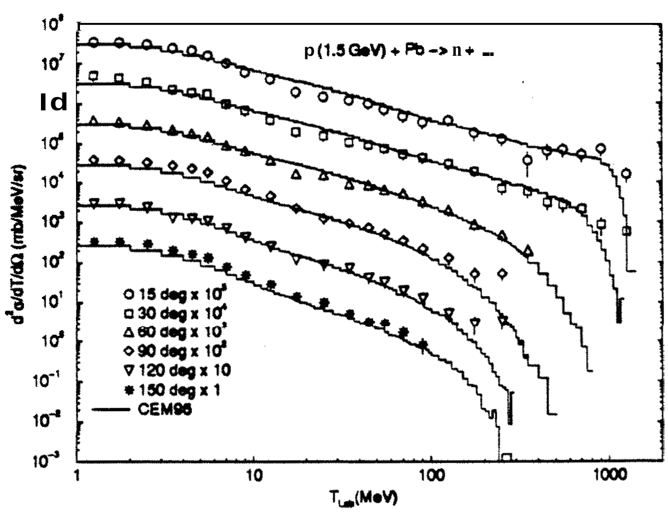
CEM95


p (1.5 GeV) + Pb -> n + ...
$d^2σ/dT/dΩ$ (mb/MeV/sr)
T_{Lab}(MeV)
○ 15 deg x 10^5
□ 30 deg x 10^4
△ 60 deg x 10^3
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* 150 deg x 1
CEM95

September 14, 1998

Simulating Accelerator Radiation Environments
Fourth Interanational Workshop (SARE4)
Hyatt Regency, Knoxville, TN, September **13-16, 1998**

Improved Cascade-Exciton Model of Nuclear Reactions

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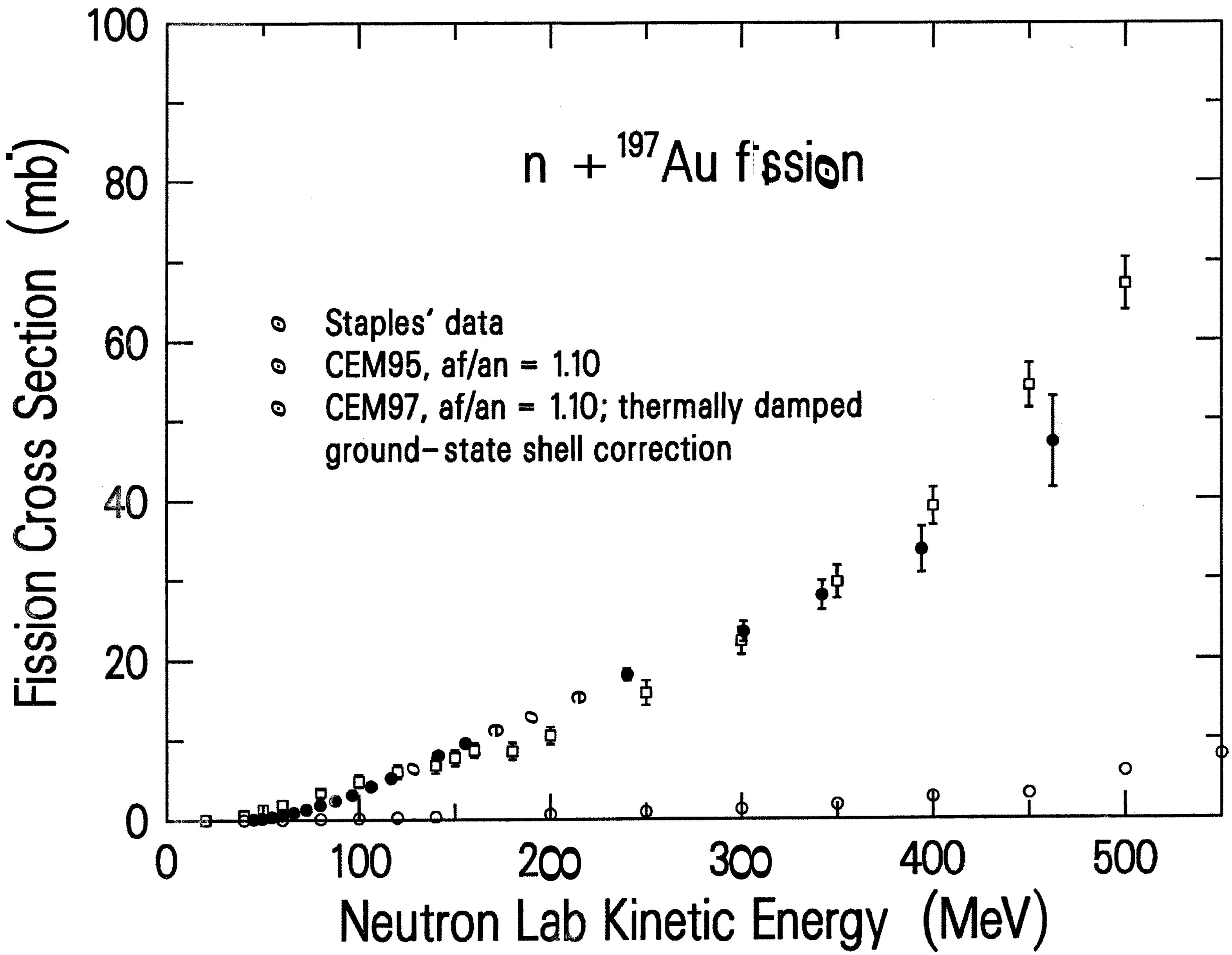
Comparison between the main assumptions of the CEM97, Bertini, and ISABEL INC models

	CEM97	Bertini	ISABEL
Method	INC + PE + EQ	INC + EQ or INC + PE + EQ	the same
INC stage	Improved Dubna INC	Bertini INC	ISABEL INC
Monte Carlo technique	"spacelike"	the same	"timelike"
Nuclear density distribution	$\rho(r) = \rho_0/\{exp[(r-c)/a]+1\}$ $c = 1.07A^{1/3}$ fm, a = 0.545 fm $\rho_n(r)/\rho_p(r) = N/Z$ $\rho(r) = \alpha_i\rho(0); i = 1,...,7$ $\alpha_1 = 0.95$, $\alpha_2 = 0.8$, $\alpha_3 = 0.5$, $\alpha_4 = 0.2$, $\alpha_5 = 0.1$, $\alpha_6 = 0.05$, $\alpha_7 = 0.01$	the same the same the same $\rho(r) = \alpha_i\rho(0); i = 1,...,3$ $\alpha_1 = 0.9$, $\alpha_2 = 0.2$, $\alpha_3 = 0.01$	the same the same the same $i = 1,...,8$
Nucleon potential	$V_N = T_F + B_N$	the same	Nucleon kinetic energy (T_N) dependent potential $V_N = V_i(1 - T_N/T_{max})$
Pion potential	$V_\pi = 25$ MeV	$V_\pi = V_N$	$V_\pi = 0$
Mean binding nucleon energy	$B_N \simeq 7$ MeV	the same	initial B_N from mass table; the same value is used throughout the calculation
Elementary cross sections	new, CEM97, last update March 1999	standard Bertini INC (old)	standard ISABEL (old)
A + A interactions	not considered	the same	allowed
γA interactions	may be considered	not considered	not considered
Condition for passing from the INC stage	$\mathcal{P} = \mid (W_{mod.} - W_{exp.})/W_{exp.} \mid$, $\mathcal{P} = 0.3$	cutoff energy ~ 7 MeV	different cutoff energies for p and n. as in VEGAS code
Nuclear density depletion	not considered	the same	considered
PE stage	Improved MEM (CEM97)	MPM (LAHET) model	the same
EQ stage	CEM97 model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	Dresner model for n, p, d, t, ^{3}He, ^{4}He emission (+ fission) (+ γ)	the same
Level density	CEM97 models for $a = a(Z, N, E')$	LAHET models for $a = a(Z, N, E')$	the same
Multifragmentation of light nuclei	Fermi breakup as in LAHET	the same	the same
Fission models	CEM model for σ_f, RAL fission fragmentation	ORNL or RAL models	the same

Comparison between the main assumptions of the **MEM (CEM97) and MPM (LAHET)**

	MEM (CEM97)	MPM (LAHET)
Master equation; computation method	**MEM** (CEM97), differs from MPM; Monte Carlo	MPM **(LAHET),** differs from MEM the same
Nuclear transitions taken into account	**An** $= +2, 0, -2$	only **An** $= +2$
. Matrix elements for nuclear transitions	**MEM** algorithm: $\|M\|^2 \sim < \sigma(v_{rel}) v_{rel} > / V_{int}$	Kalbach parameterization
Pauli correction term	$A = (p^2 + h^2 + p - h)/4 - h/2$	$A = E_{Pauli} - [p(p+1) + h(h+1)]/4g_0$
Multiple particle emission	allowed, **no** limitation	the same
Type of particle considered	n, **p**, d, t, ^{3}**He**, ^{4}**He**	the same
Level density parameter, $g = 6a(A, Z, E^*)/\pi^2$	**CEM97** parameterization (+ **9 CEM95** options)	Ignatyuk (from **GNASH)**
Inverse cross sections	Dostrovsky	Kalbach parameterization
Coulomb barriers	Dostrovsky form ($r_0 = 1.5$ fm)	Kalbach form ($r_0 = \mathbf{1.7}$ fm)
Angular distribution of preequilibrium particles	forward picked, **CEM** algorithm: either by Master equation or from kinematics	initially, isotropic; Kalbach parameterization may be applied later



n + 197Au fission
Staples' data
CEM95, af/an = 1.10
CEM97, af/an = 1.10; thermally damped ground-state shell correction
Fission Cross Section (mb)
Neutron Lab Kinetic Energy (MeV)
0
20
40
60
80
100
0
100
200
300
400
500

Cross Sections of Spallation Residues Produced in 1A GeV ^{208}Pb on Proton Reactions

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Spallation residues produced in 1 GeV per nucleon ^{208}Pb on proton reactions have been studied using the Fragment Separator facility at GSI. Isotopic production cross sections of elements from $_{61}$Pm to $_{82}$Pb have been measured down to 0.1 mb with a high accuracy. The recoil kinetic energies of the produced fragments were also determined. The obtained cross sections agree with most of the few existing gamma-spectroscopic data. The data are compared with different intranuclear-cascade and evaporation-fission models. Drastic deviations were found for a standard code used in technical applications.

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Spallation reactions have recently captured an increasing interest due to their technical applications as intense neutron sources for accelerator-driven subcritical reactors [1] or spallation neutron sources [2]. The design of an accelerator-driven system (ADS) requires precise knowledge of nuclide production cross sections in order to be able to predict the amount of radioactive isotopes produced inside the spallation target. Indeed, short-lived isotopes may be responsible for maintenance problems and long-lived ones will increase the long term radiotoxicity of the system. Recoil kinetic energies of the fragments are important for studies of radiation damages in the structure materials or in the case of a solid target. Data concerning lead are particularly important since in most of the ADS concepts actually discussed, lead or lead-bismuth alloy is considered as the preferred material of the spallation target.

The present experiment, using inverse kinematics, is able to supply the identification of all the isotopes produced in spallation reactions and information on their recoil velocity. Moreover, the data represent a crucial benchmark for the existing spallation models used in the ADS technology. The precision of these models to estimate residue production cross sections is still far from the performance required for technical applications, as it was shown in Ref. [3]. This can be mostly ascribed to the lack of complete distributions of all produced isotopes to constrain the models. The available data were generally obtained by chemistry or gamma spectroscopy [4–6] which give access mostly to cumulative yields produced after long chains of decaying isotopes.

In this Letter, we report on complete isotopical production cross sections for heavy fragments produced in spallation of ^{208}Pb on proton at 1A GeV, down to 0.1 mb with a high precision. The kinematic properties of the residues are also studied. The cross sections of lighter isotopes produced by fission will be presented in a forthcoming publication.

The experimental method and the analysis procedure have been developed and applied in previous experiments [7–9]. The primary beam of 1A GeV ^{208}Pb was delivered by the heavy-ion synchrotron SIS at GSI, Darmstadt. The proton target was composed of 87.3 mg/cm^2 liquid hydrogen [IO] enclosed between thin titanium foils of a total thickness of 36 mg/cm^2. The primary-beam intensity was continuously monitored by a beam-intensity monitor (SEETRAM) based on secondary-electron emission. In order to subtract the contribution of the target windows from the measured reaction rate, measurements were repeated with the empty target. Heavy residues produced in the target were all strongly forward focused due to the inverse reaction kinematics. They were identified using the Fragment Separator (FRS) [11].

The FRS is a two-stage magnetic spectrometer with a dispersive intermediate image plane (S_2) and an achromatic final image plane (S_4) with momentum acceptance of 3% and angular acceptance of 14.4 mrad around the beam axis. Two position-sensitive plastic scintillators placed at S_2 and S_4, respectively, provided the magnetic-rigidity $(B\rho)$ and time-of-flight measurements, which allowed to determine the mass-over-charge ratio of the particles. In the analysis, totally stripped residues were considered only. In the case of residues with the highest nuclear charges (above $_{65}$Tb) an achromatic degrader (5.3 to 5.9 g/cm^2 of aluminum) was placed at S_2 to obtain a better Z resolution. The elements below terbium were identified from an energy-loss measurement in an ionization chamber (MUSIC). The velocity of the identified residue was determined at S_2 from the $B\rho$ value and transformed into the frame of the beam in the middle of the target taking into account the appropriate energy loss. About 100

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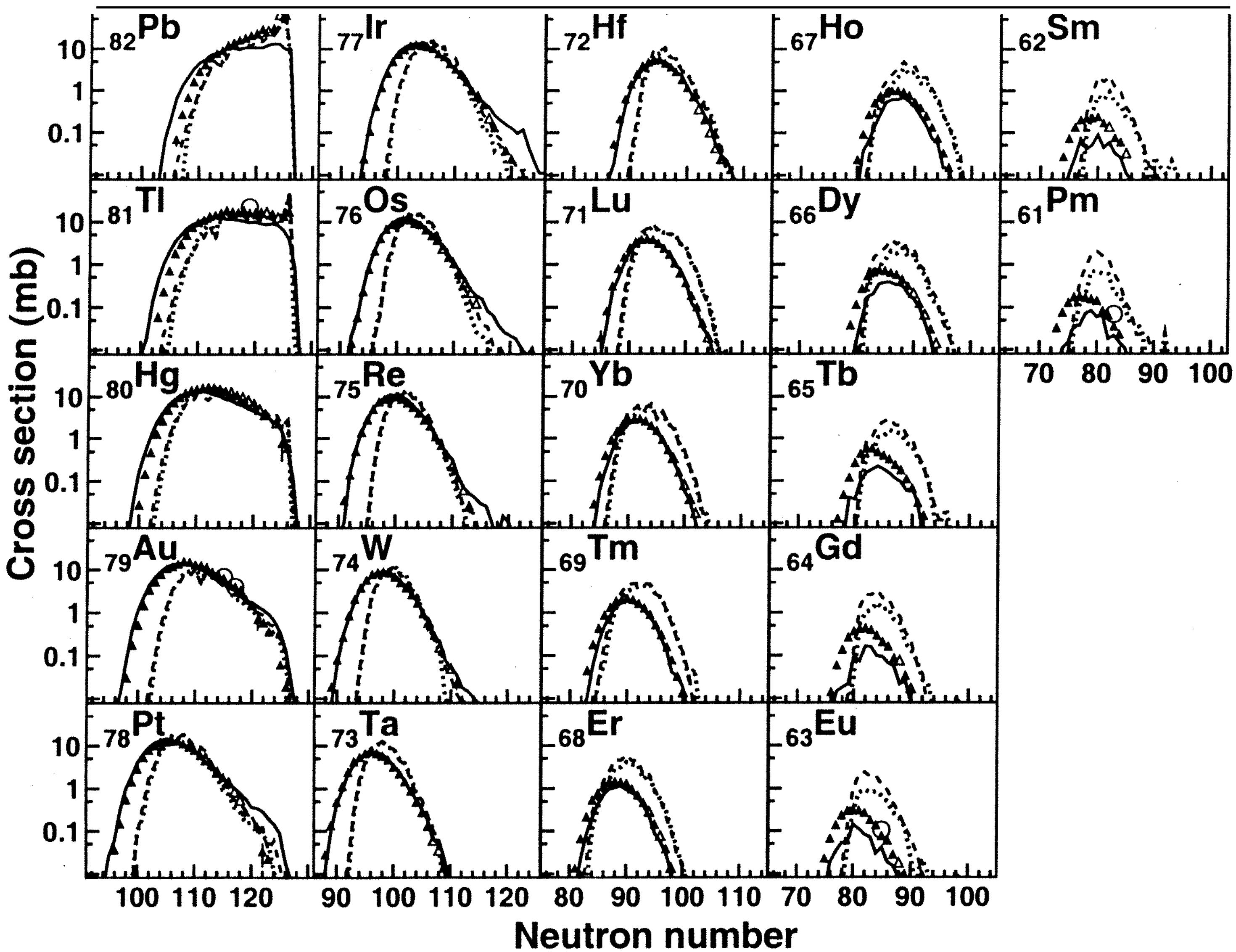


FIG. 2. Isotopic production cross-sections of elements between Z=82 and 61, in the reaction of 1·A GeV ^{208}Pb on hydrogen, versus neutron number. Stable (resp. radioactive) isotopes are marked by open (resp. full) triangles. Gamma-spectroscopy data regarding shielded isotopes from [6] are plotted as open circles. The solid, dashed and dotted curves were calculated with the Cugnon-Schmidt [20,21], Bertini [16]-Dresner [18,19] and Isabel [17]-Dresner models, respectively.

cross-section is the sum of the production of the ground and the isomeric states. The data agree within their error bars, except for the isotope with the lowest cross-section

to the fact that the prediction of the neutron-proton evaporation competition in the Dresner code is not satisfying. The magnitude of the measured and calculated

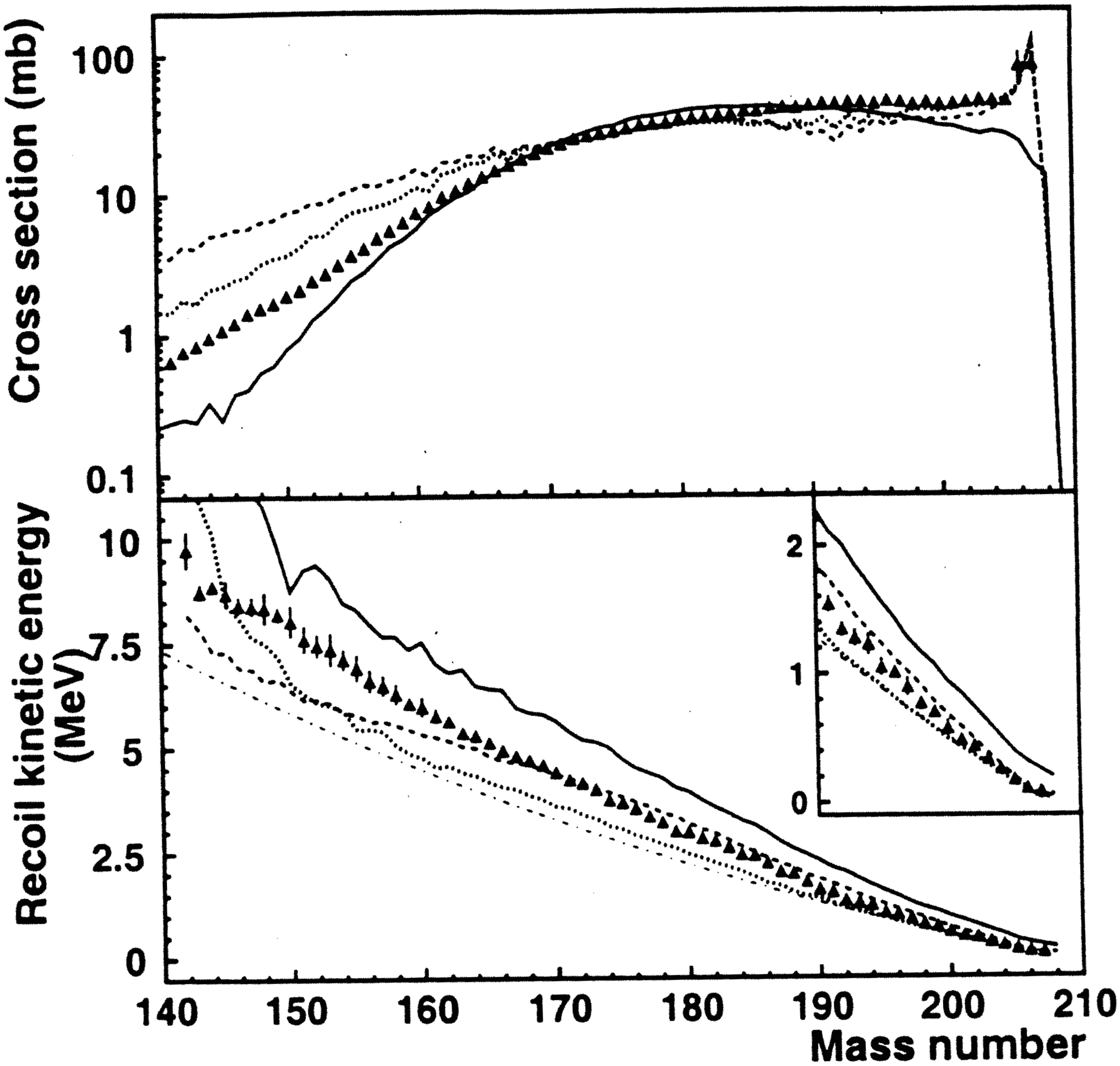
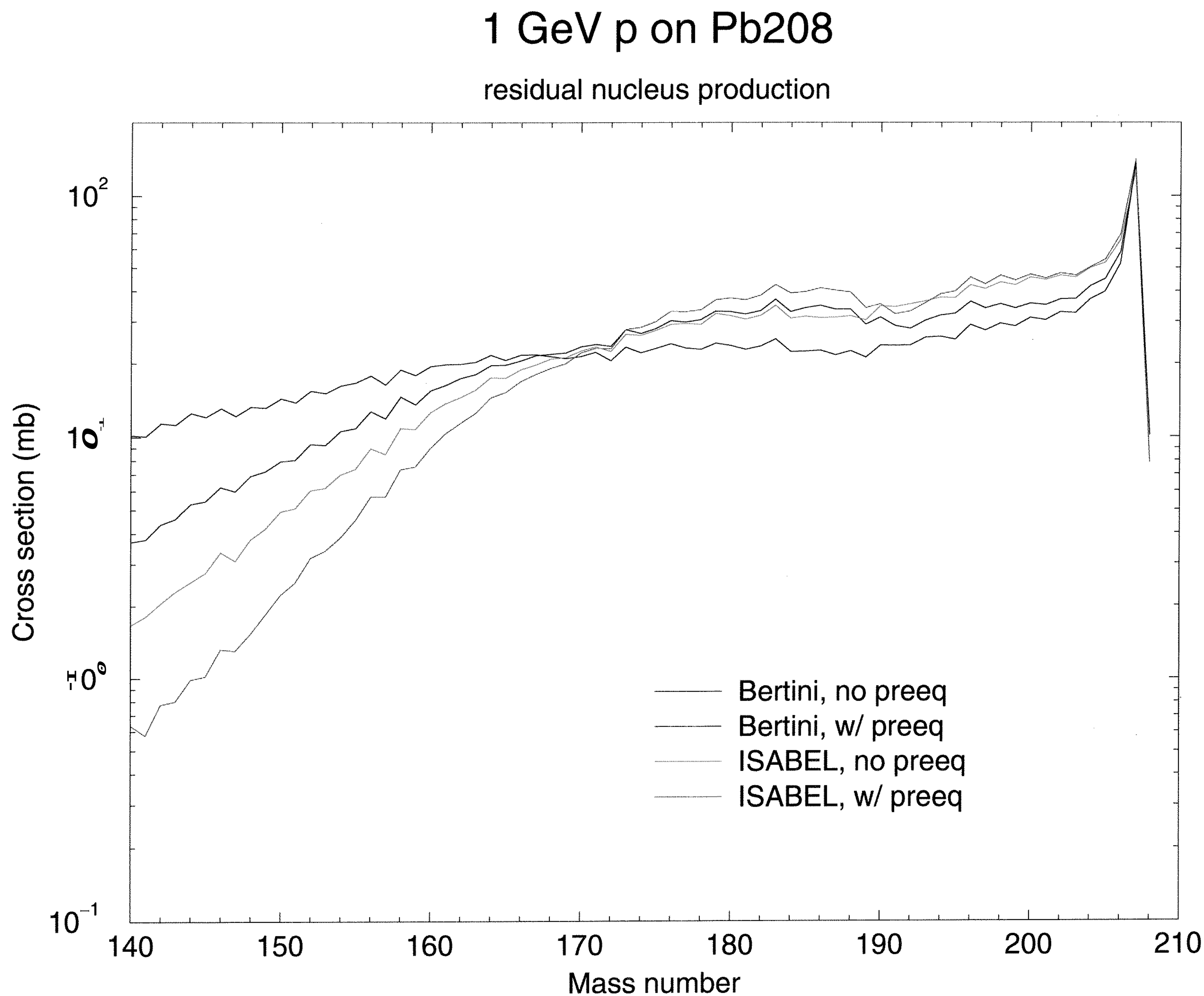


FIG. 3. Mass distribution (upper panel) and recoil kinetic energy (bottom panel) of the residues produced in 1·A GeV ^{208}Pb on hydrogen reactions (triangles) versus mass number, compared with the Cugnon-Schmidt (solid line), Bertini-Dresner (dashed line) and Isabel-Dresner (dotted line) models. The dash-dotted line shows the recoil kinetic energies expected from the Morrissey systematics [23].

The velocity distribution of each residue was also determined, from which it was possible to infer information about the recoil kinetic energy in the projectile system. In the bottom part of Fig. 3 the


1 GeV p on Pb208
residual nucleus production
Cross section (mb)
Mass number
10^2
10^1
10^0
10^-1
140
150
160
170
180
190
200
210
Bertini, no preeq
Bertini, w/ preeq
ISABEL, no preeq
ISABEL, w/ preeq

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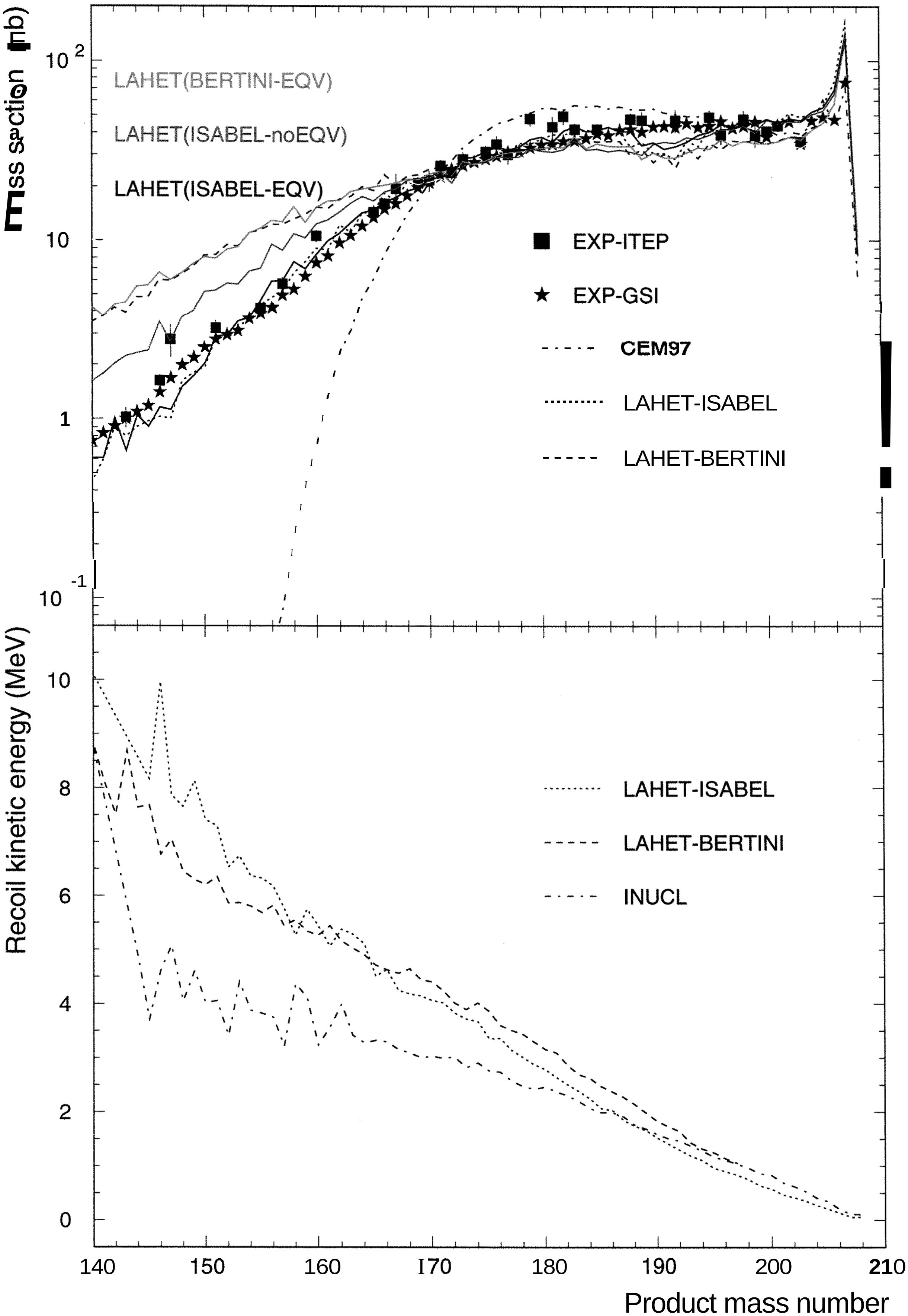
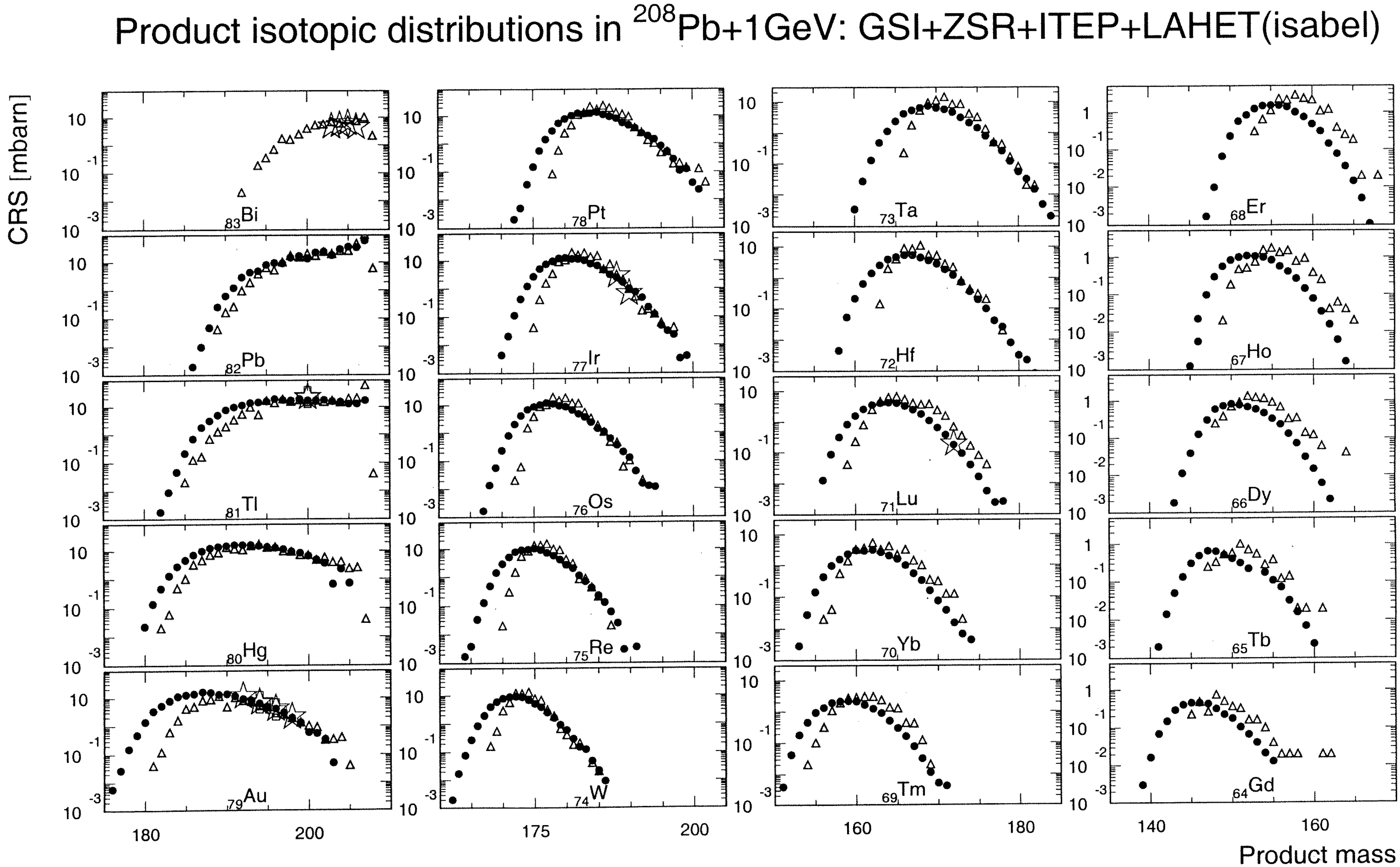
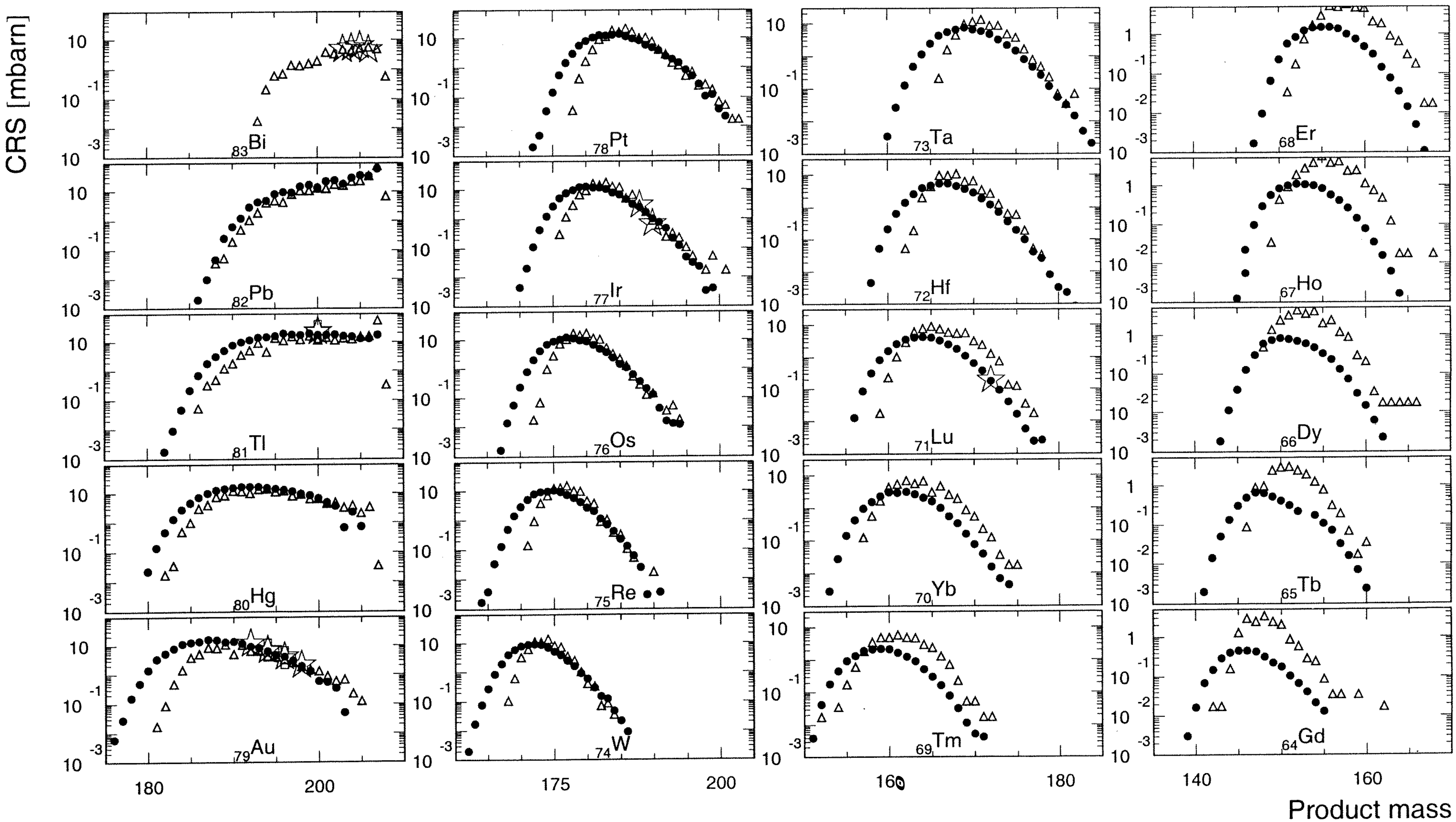
Mass yields in Pb-208 irradiated with 1GeV protons



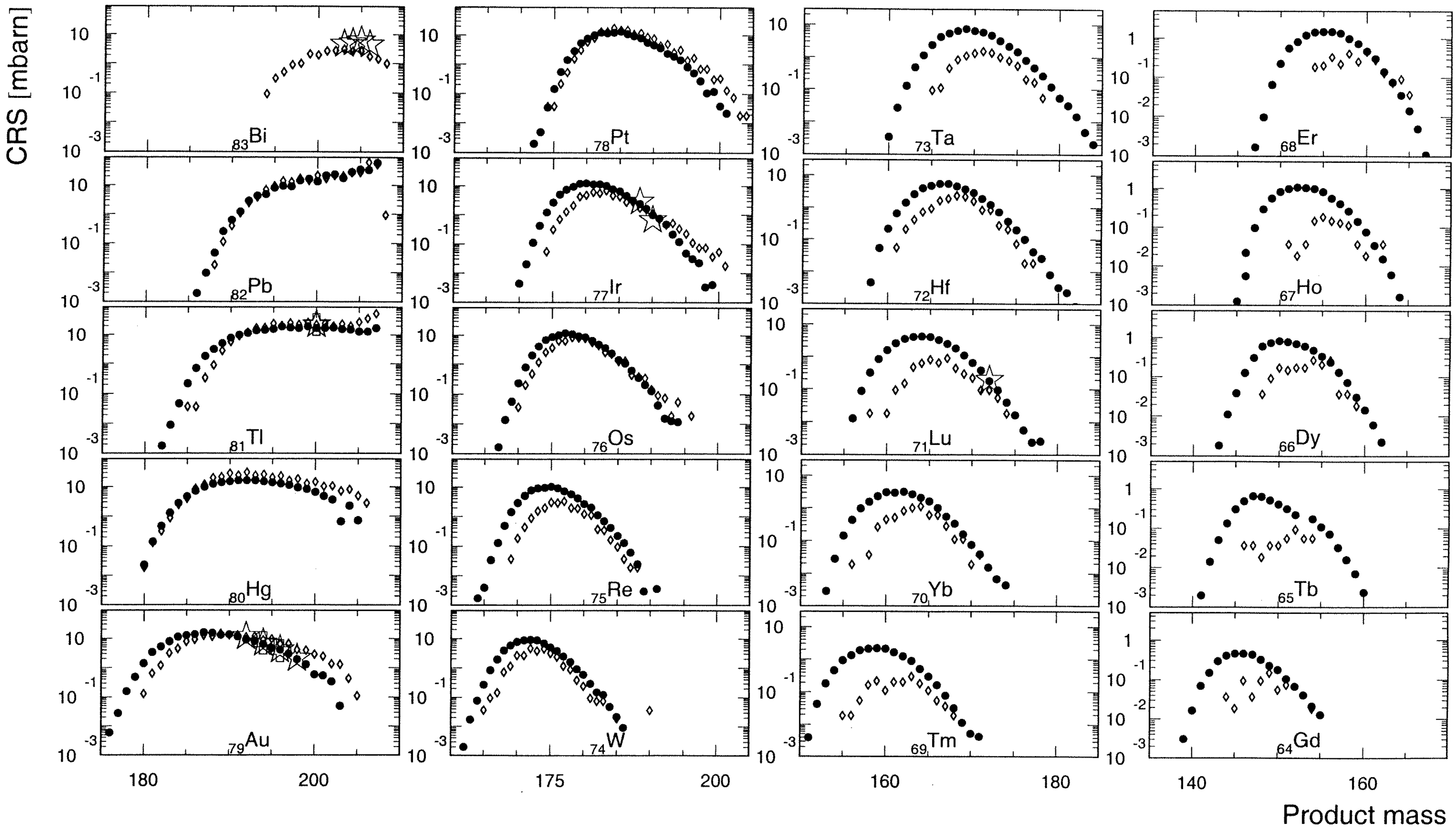


Product isotopic distributions in ^{208}Pb+1GeV: GSI+ZSR+ITEP+LAHET(isabel)
CRS [mbarn]
Product mass
$_{83}$Bi
$_{82}$Pb
$_{81}$Tl
$_{80}$Hg
$_{79}$Au
$_{78}$Pt
$_{77}$Ir
$_{76}$Os
$_{75}$Re
$_{74}$W
$_{73}$Ta
$_{72}$Hf
$_{71}$Lu
$_{70}$Yb
$_{69}$Tm
$_{68}$Er
$_{67}$Ho
$_{66}$Dy
$_{65}$Tb
$_{64}$Gd

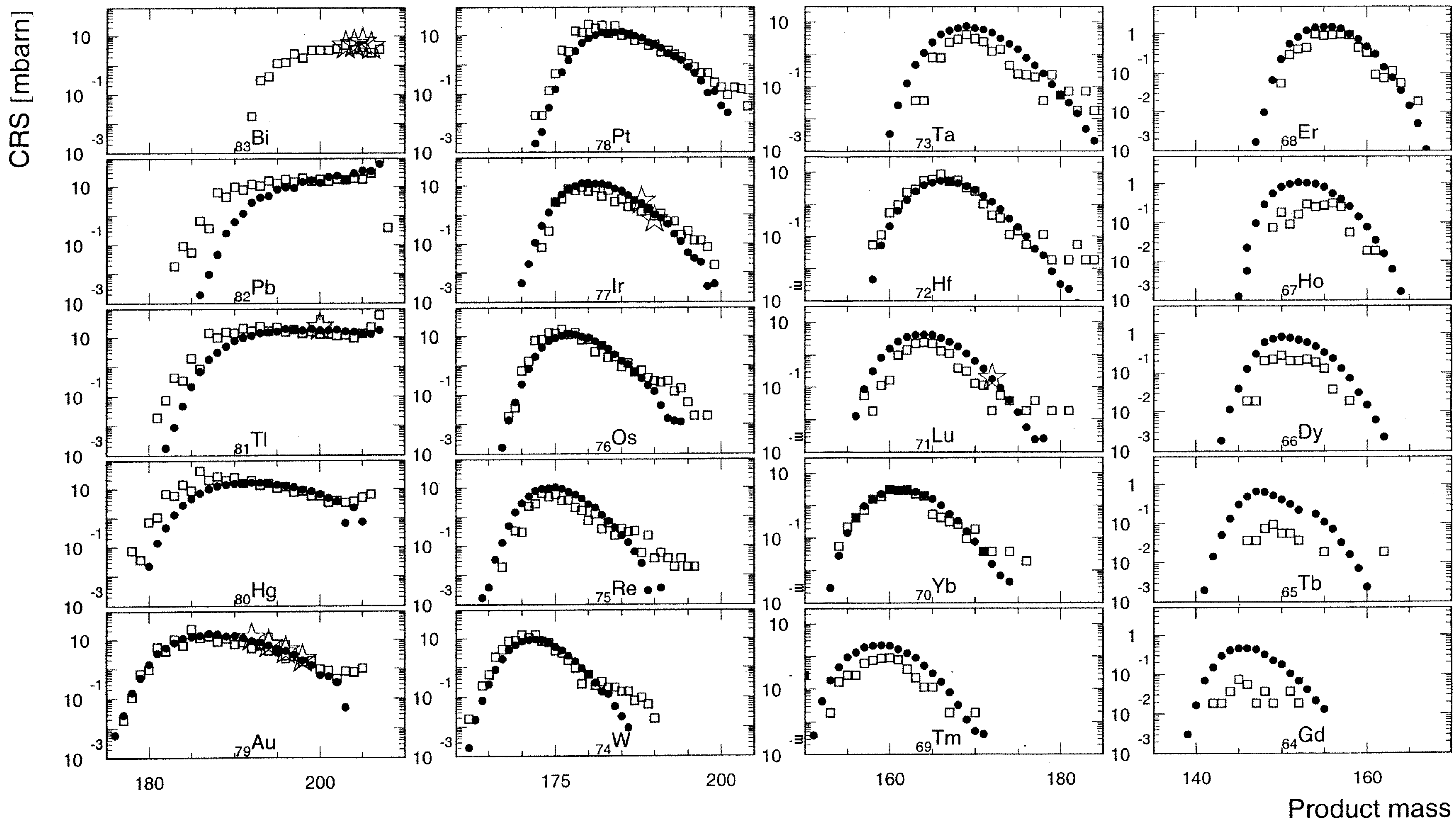
Product isotopic distributions in ^{208}Pb+1GeV: GSI+ZSR+ITEP+LAHET(bertini)



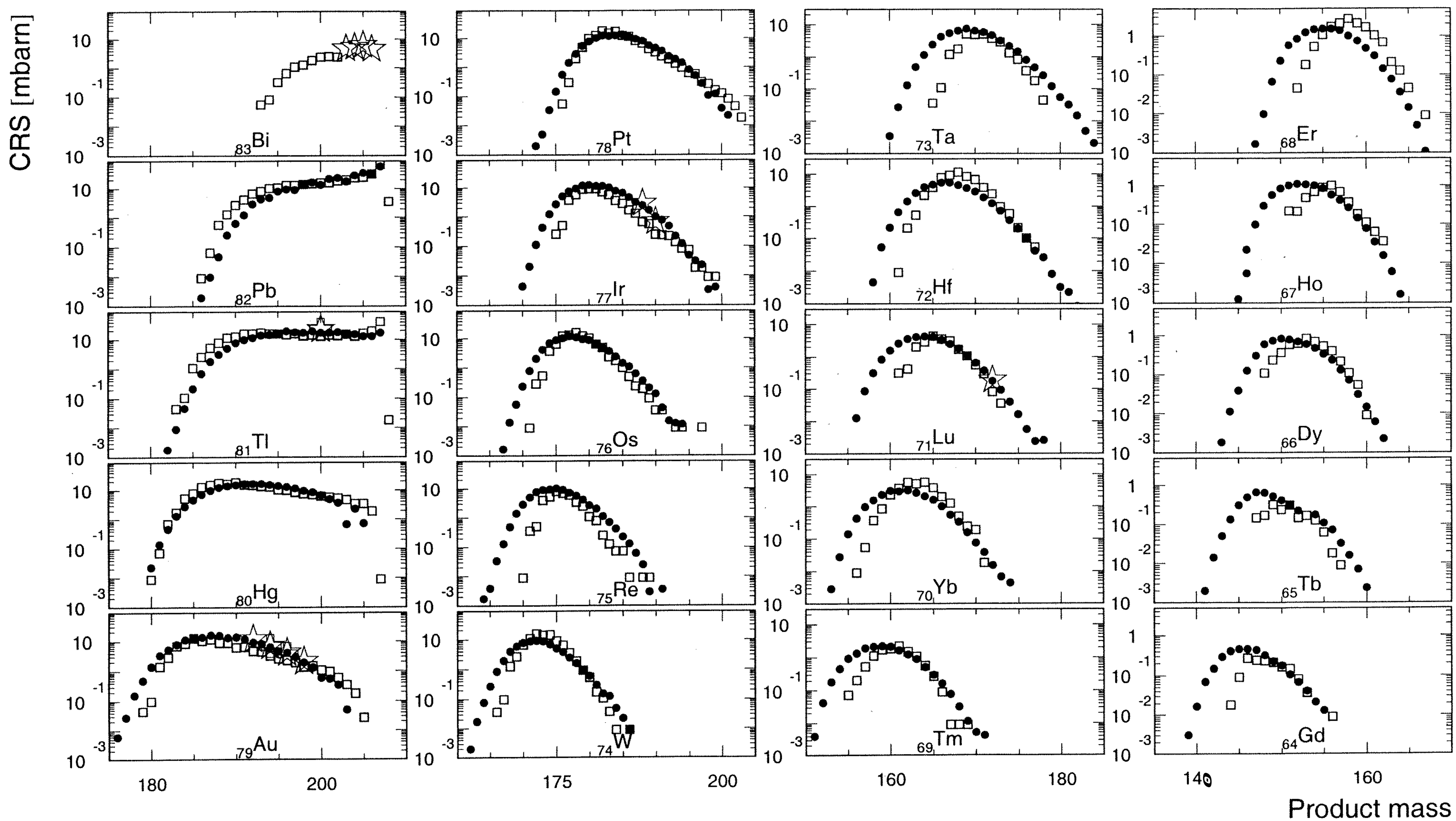
Product isotopic distributions in ^{208}Pb+1GeV: GSI+ZSR+ITEP+INUCL



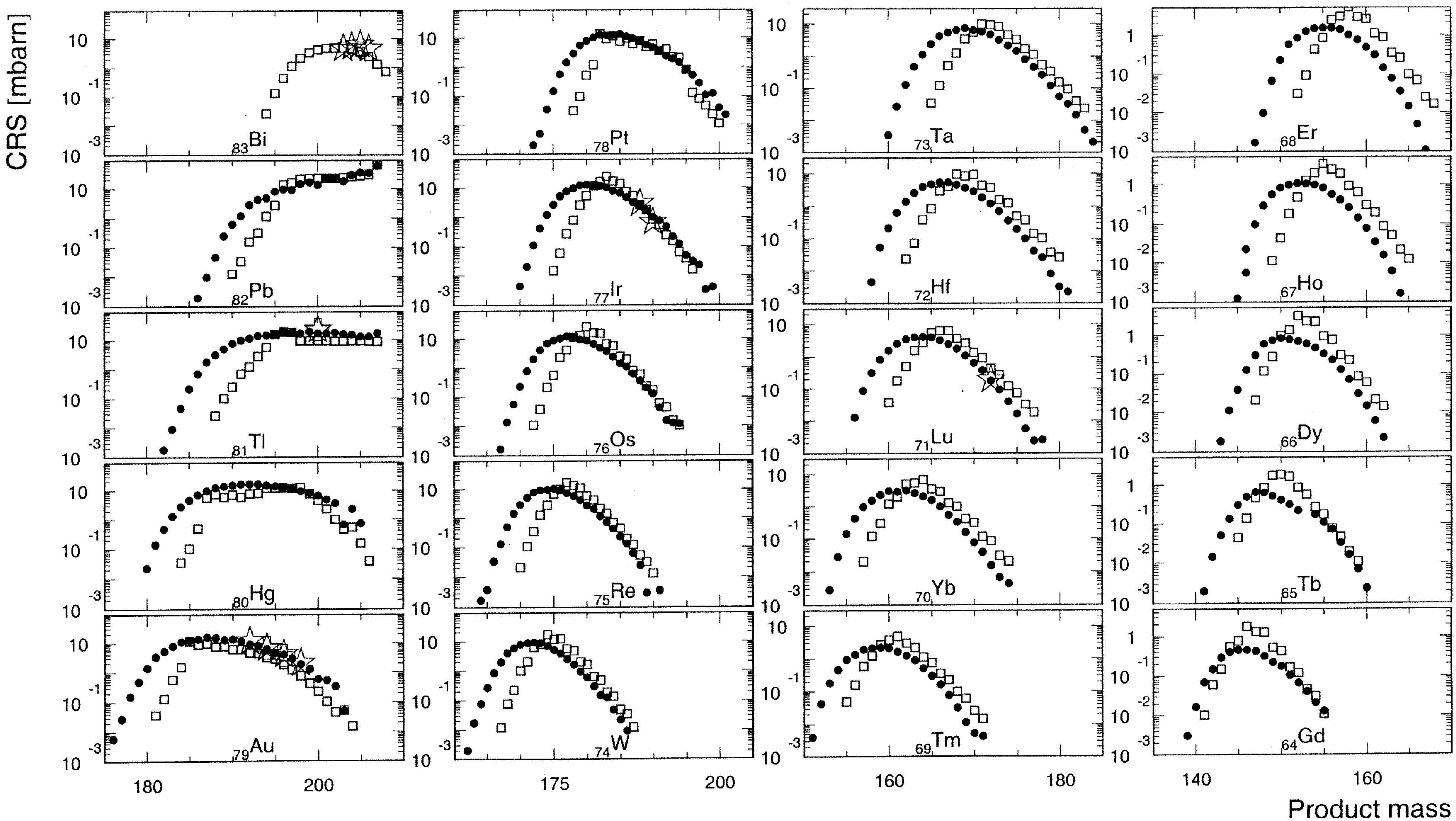
Product isotopic distributions in ^{208}Pb+1GeV: GSI+ZSR+ITEP+CASCADE



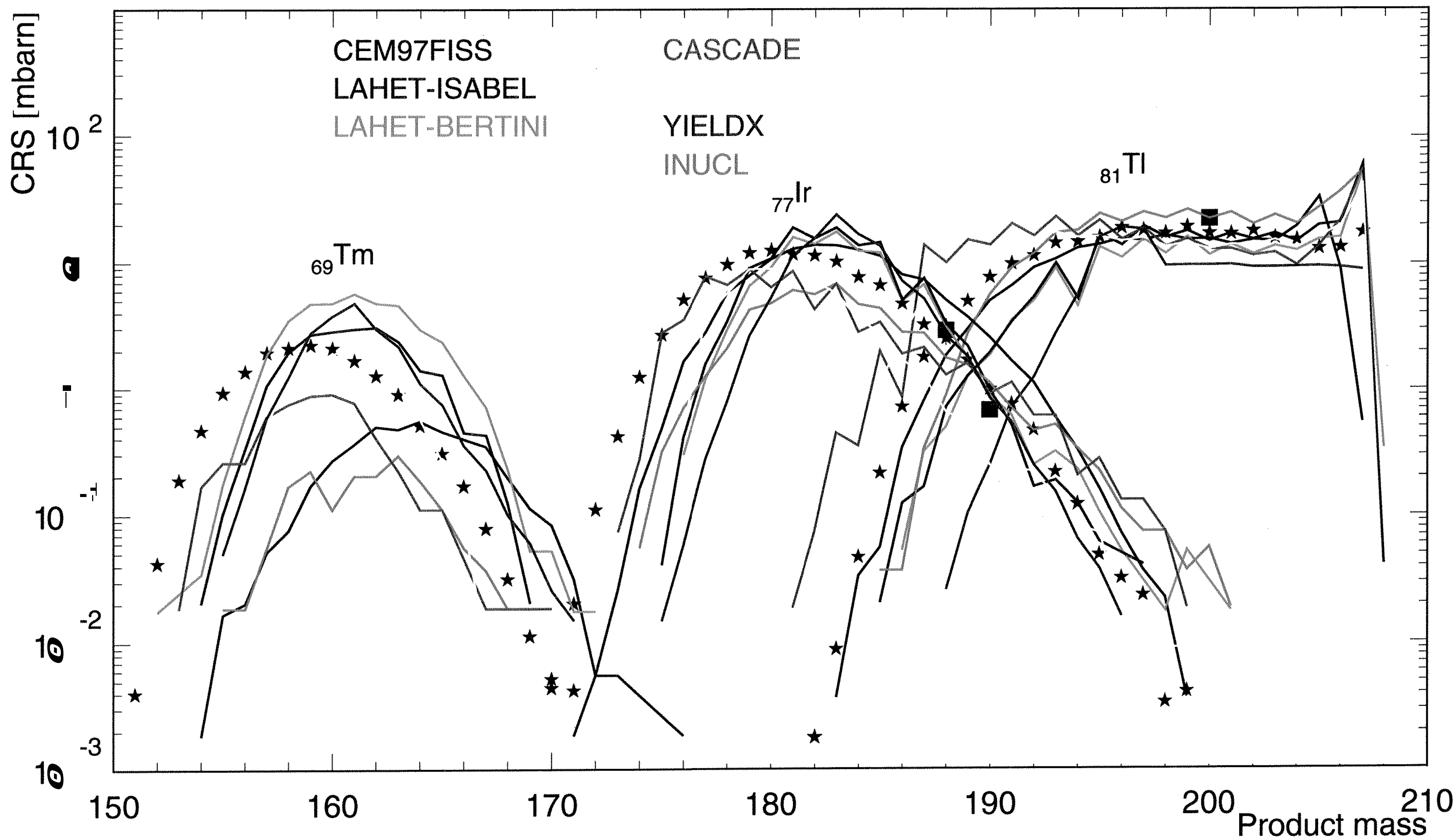
Product isotopic distributions in ^{208}Pb+1GeV: GSI+ZSR+ITEP+CASCADE(inpe)



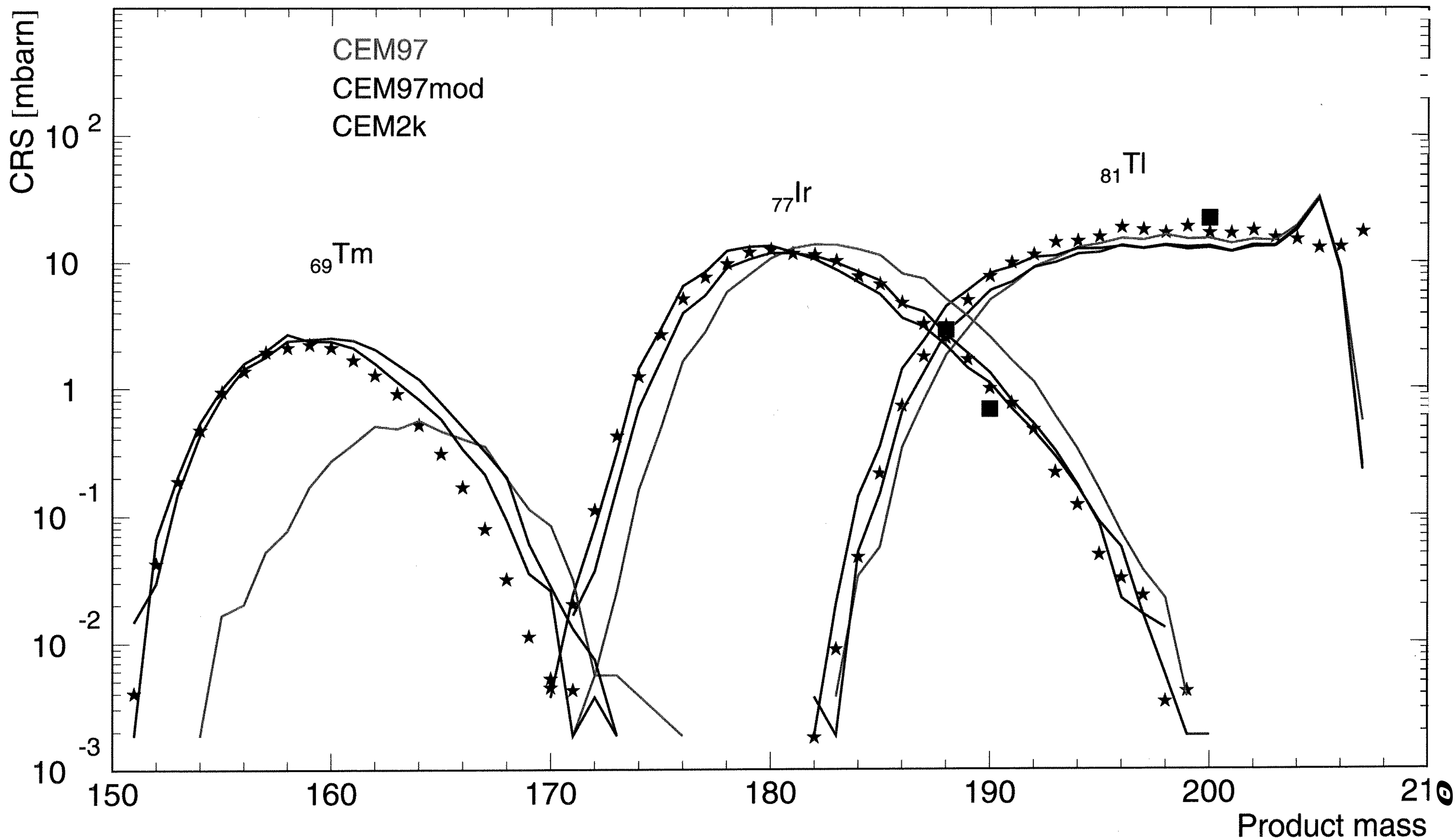
Product isotopic distributions in ^{208}Pb+1GeV: GSI+ZSR+ITEP+YIELDX



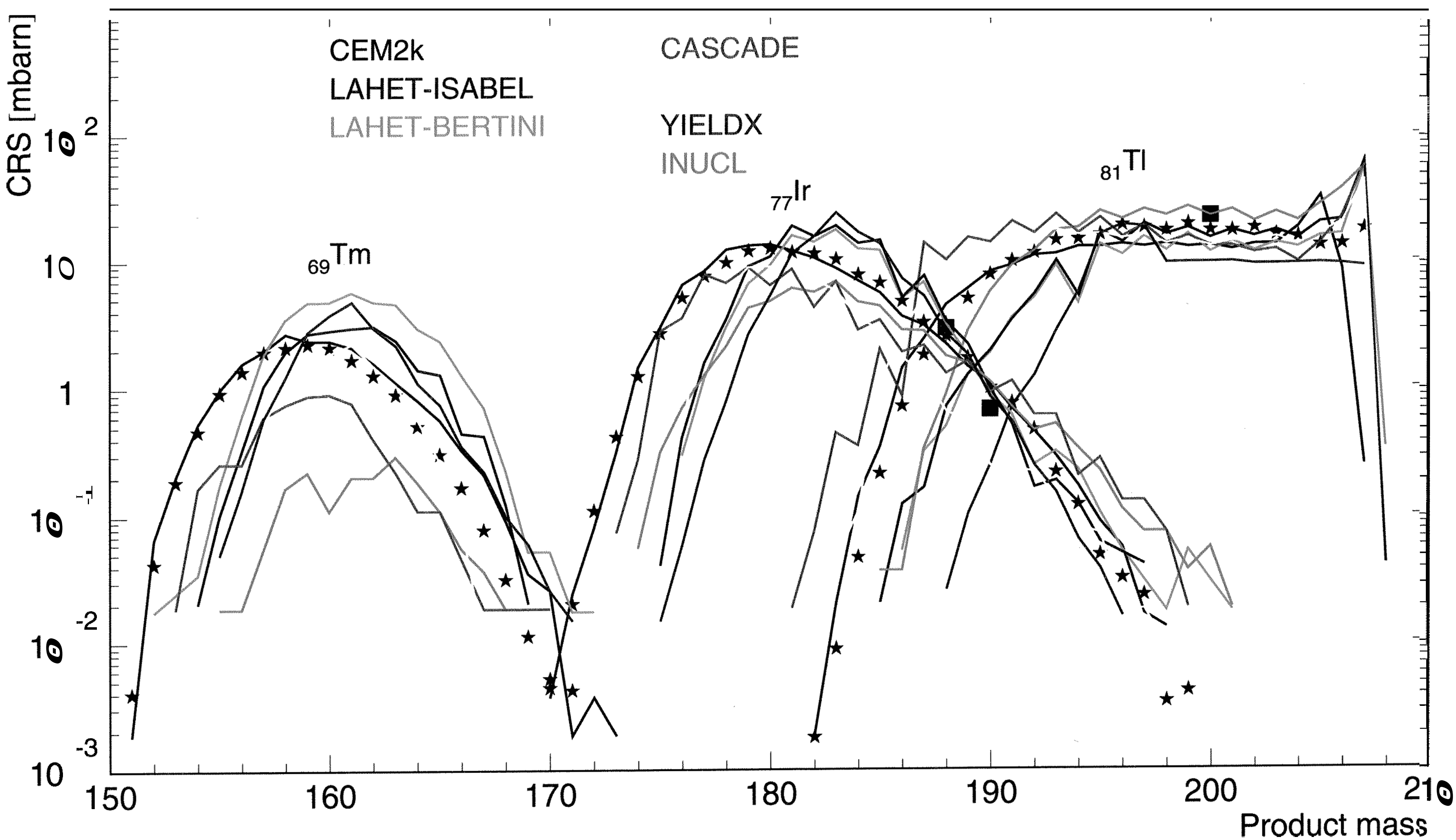
Isotopic distributions of the products in Pb-208+1GeV protons: GSI+ITEP+Codes



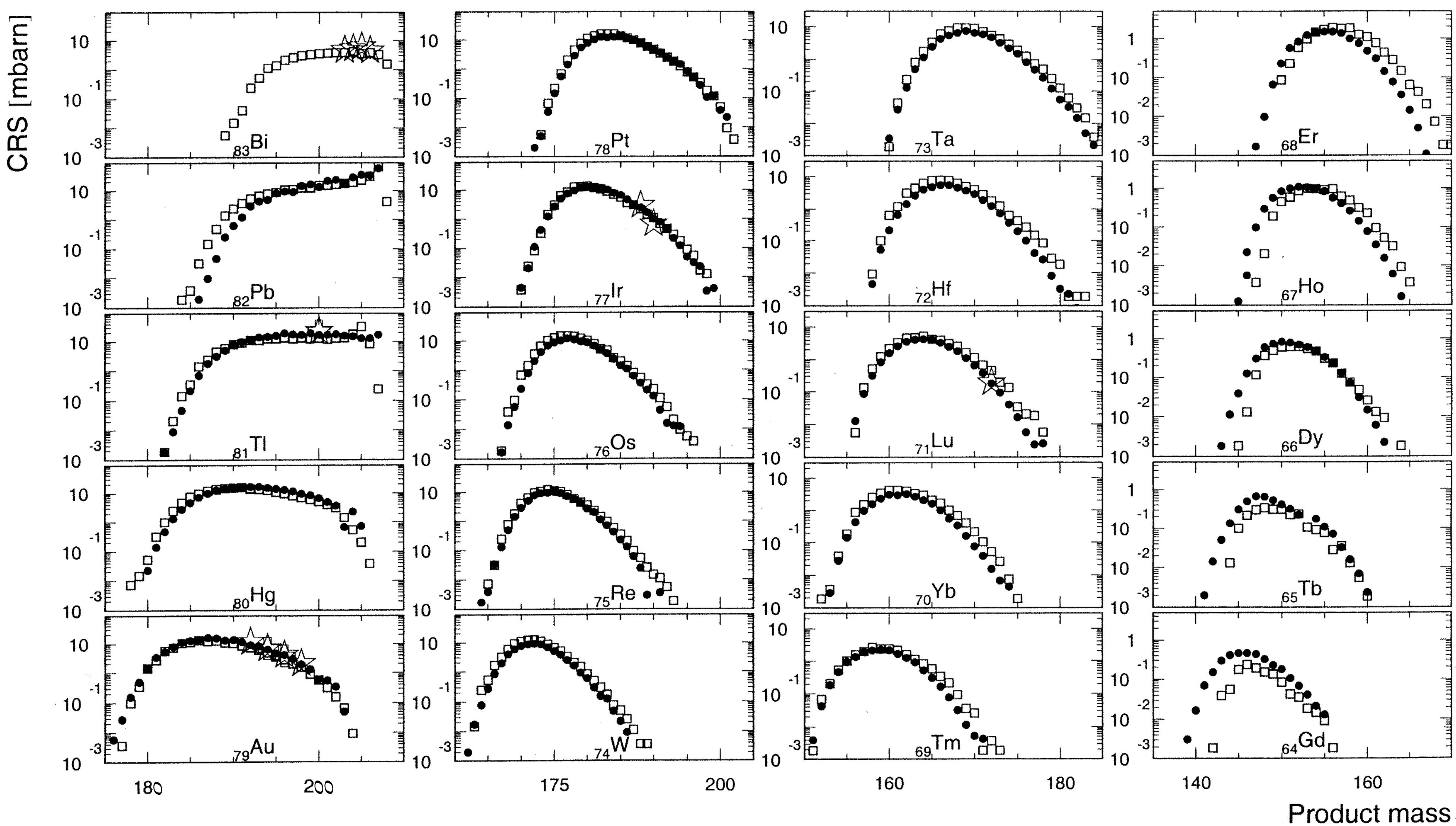
Isotopic distributions of the products in Pb-208+1GeV protons: GSI+ITEP+Codes



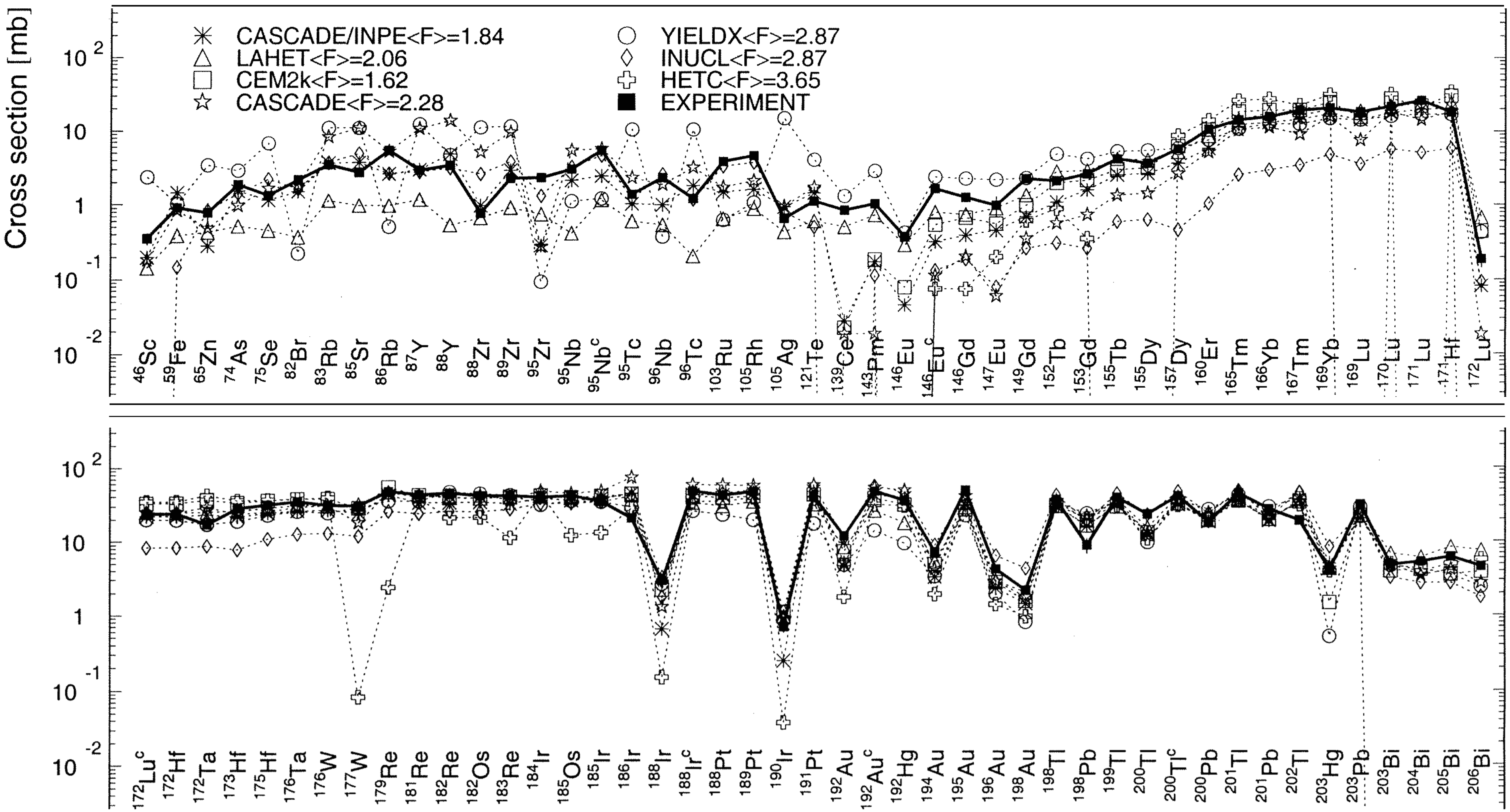
Isotopic distributions of the products in Pb-208+1GeV protons: GSI+ITEP+Codes



Product isotopic distributions in ^{208}Pb+1GeV: GSI+ZSR+ITEP+CEM2k



Products in Pb-208 irradiated with 1GeV protons



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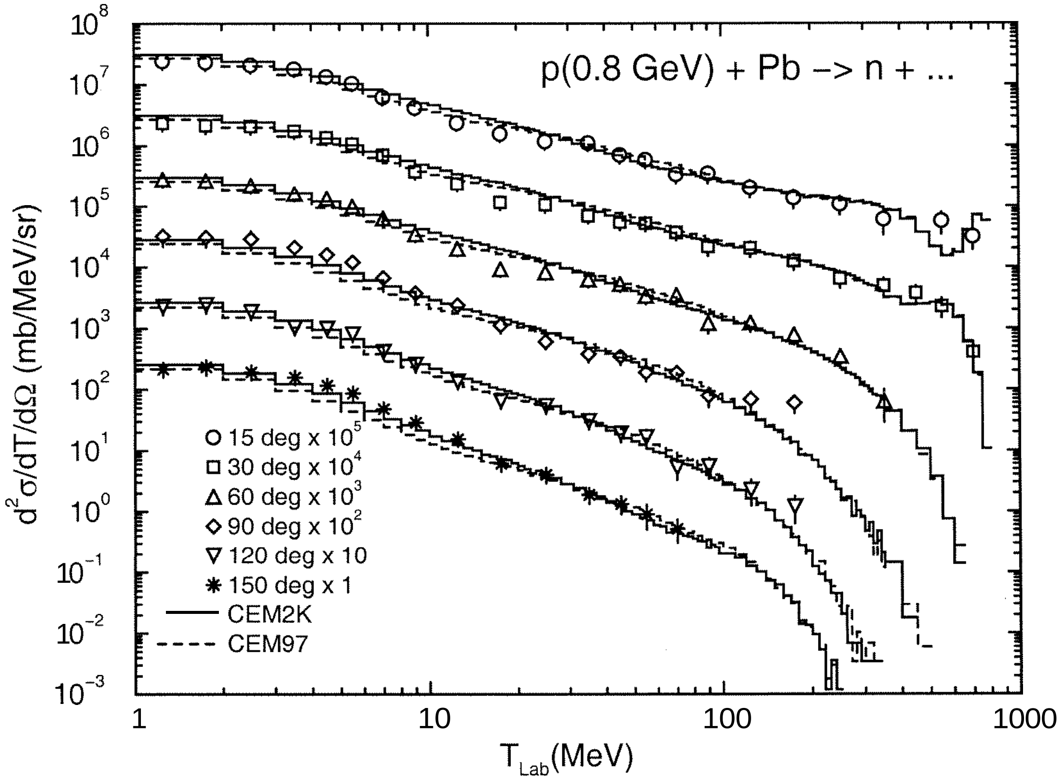
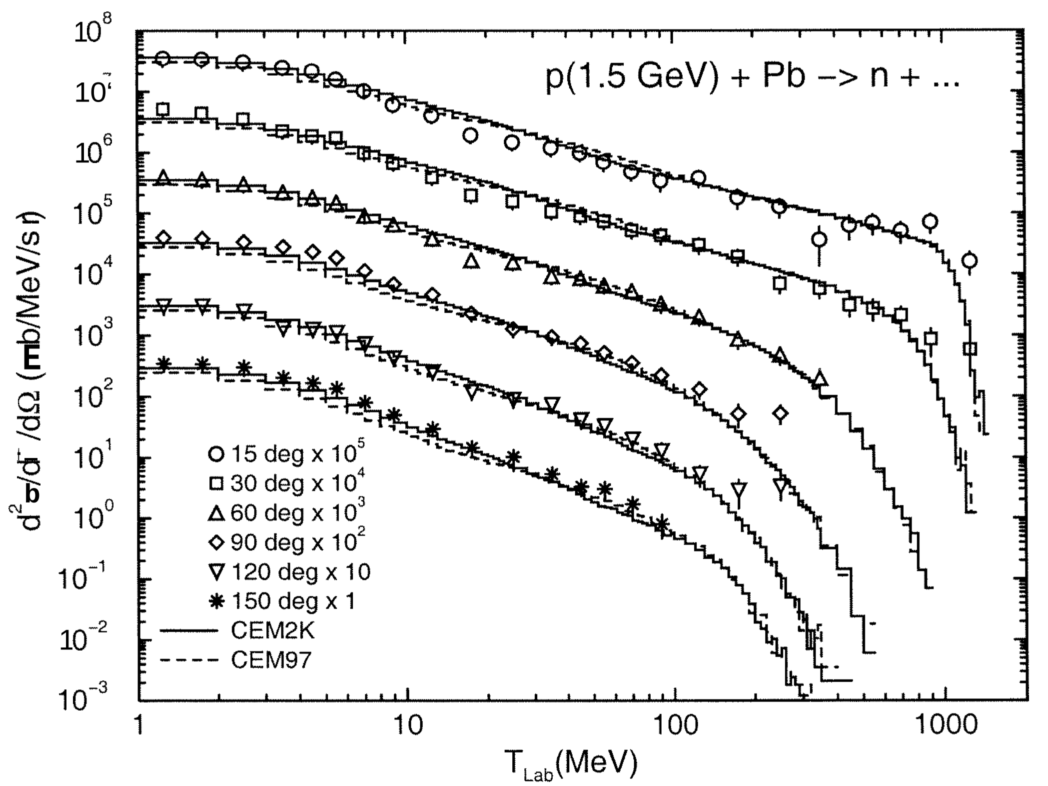

p(0.8 GeV) + Pb –> n + ...
15 deg x 10^5
30 deg x 10^4
60 deg x 10^3
90 deg x 10^2
120 deg x 10
150 deg x 1
CEM2K
CEM97
d²σ/dT/dΩ (mb/MeV/sr)
T_{Lab}(MeV)


p(1.5 GeV) + Pb –> n + ...
15 deg x 10^5
30 deg x 10^4
60 deg x 10^3
90 deg x 10^2
120 deg x 10
150 deg x 1
CEM2K
CEM97
T_{Lab}(MeV)

Further work

- fission cross sections
- fission fragment A-, Z-, T-, E^*-, L-distributions
- inverse cross sections
- complex particle and fragment emission
- where to stop evaporation, at
  A = 4 (most models),
  A = 18 (Botvina, Shmakov, Uzhinsky'95),
  A = 20 (Schmidt'98),
  A = 28 (Furihata'00),
  or even further ?
- criteria for transaction from INC to PE and from PE to EV
- do we need to use in-medium elementary cross sections, and where to take them from ?
- reliable optical potential for all particles, not only nucleons
- ...