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R-MATRIX AND RR-MATRIX CALCULATIONS FOR CROSS SECTIONS FOR PHOTOIONIZATION OF OUTERMOST SUBSHELL IN NOBILE GAS ATOMS

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Abstract

Photon impact integral ionization cross section (σ) as well as photoelectron asymmetry parameter (β) for the reactions $h\nu + Ne(1s^2\ 2s^2\ 2p^6) \rightarrow Ne^+(1s^2\ 2s^2\ 2p^5) + e^-$, $h\nu + Ar(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6) \rightarrow Ar^+(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5) + e^-$, $h\nu + Kr(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6) \rightarrow Kr^+(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^5) + e^-$ and $h\nu + Xe(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^6) \rightarrow Xe^+(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^2\ 4p^6\ 4d^{10}\ 5s^2\ 5p^5) + e^-$ have been calculated in the L-S and j-j coupling schemes using Hartree-Fock (HF) wavefunctions within the reliable non-relativistic R-matrix as well as relativistic R-matrix (RR-matrix) methods in both the length and velocity gauges in the energy range of experimental data available. Comparison is made with all available experimental data as well as other theoretical results. Our present theoretical investigation clearly demonstrates that there is a good agreement between our present R-matrix results and RR-matrix results as well as with other results in the case of neon which reflects that the correlation and relativity are not important in this case, in the energy range of present consideration. Whereas in the case of xenon (Z=54), the independent-particle approximation completely breaks down, i.e., HF cross sections are both qualitatively as well as quantitatively incorrect in the entire energy range which exhibit that the multielectron correlation as well as relativity are both important but interchannel interactions are more important than the intrachannel interaction and relativity for obtaining high precision results.

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Introduction

Interaction between matter and radiation corresponding to photoionization is a fundamental process of nature and of major importance which occurs everywhere in the universe.
Photoionization of matter was the first in a series of experimental discoveries followed by a corresponding theoretical explanation which led to the foundation of quantum physics. It was in fact Einstein's interpretation of the photoelectric effect that proved the concept of energy quantization by Planck to be generally valid. Despite this early success it took more than 40 years until photoelectron spectroscopy became a growing field of scientific research and finally, an analytical tool for industrial research. This was because the early efforts to record line spectra in measurements of the photoelectric effect were hampered by experimental difficulties such as insufficient energy resolution. Only after the pioneering work of the Uppsala group did photoelectron spectroscopy become a powerful tool for studying the electronic structure of matter and its chemical composition.
Accurate calculations of photoionization cross sections of atoms, molecules, clusters, solids, and ions are useful in a variety of investigations in laser physics, plasma physics, astrophysics, space physics, fusion research, etc. It is particularly useful in the context of flashlamp photopumping schemes for X-ray lasers. Most of the existing calculations of photoionization cross sections are performed employing independent particle model (IPM). In this model, the energy-level and wavefunction of the target are first calculated using the Hartree-Fock method. The interaction of the incident electromagnetic radiation with the target is treated via the first order perturbation theory. There are several theoretical methods as well as computer codes for photoionization processes in atoms, molecules and ions available in the literature. For the non-relativistic photoionization cross section, close-coupling (CC), quantum defect theory (QDT), multi-channel quantum defect theory (MQDT), density function method (DFM), local density random phase approximation (LDRPA), time dependent local density approximation (TDLDA), many body perturbation theory (MBPT), random phase approximation (RPA) and R-matrix have been used extensively [1-228]. For relativistic photoionization cross sections, relativistic R-matrix (RR-matrix), relativistic many body perturbation theory (RMBPT), Dirac atomic R-matrix code (DARC) and relativistic random phase approximation with exchange (RRPAE) have been employed in many cases. For the non-relativistic as well as relativistic structure calculations, CIV3, superstructure (SS), multiconfiguration Hartree-Fock (MCHF), Cowan, Bates, SMART, multiconfiguration Dirac-Fock (MCDF), GRASP, RRPAE and RPA computer codes have been used widely. In our present work, we have used R-matrix and RR-matrix methods for calculations of photoionization cross section and photoelectron asymmetry parameter in the case of noble gas atoms Ne, Ar, Kr and Xe.
Photon impact integral ionization cross section (σ) as well as photoelectron asymmetry parameter (β) for the reactions $h\nu+\mathrm{Ne}(1s^2\,2s^2\,2p^6) \rightarrow \mathrm{Ne}^+(1s^2\,2s^2\,2p^5) + e^-$, $h\nu+\mathrm{Ar}(1s^2\,2s^2\,2p^6\,3s^2\,3p^6) \rightarrow \mathrm{Ar}^+(1s^2\,2s^2\,2p^6\,3s^2\,3p^5) + e^-$, $h\nu+\mathrm{Kr}(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^6) \rightarrow \mathrm{Kr}^+(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^5) + e^-$ and $h\nu+\mathrm{Xe}(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^6\,4d^{10}\,5s^2\,5p^6) \rightarrow \mathrm{Xe}^+(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^6\,4d^{10}\,5s^2\,5p^5) + e^-$ have been calculated in the L-S and j-j coupling schemes using Hartree-Fock (HF) wavefunctions within the reliable non-relativistic R-matrix as well as relativistic R-matrix (RR-matrix) methods in both the length and velocity gauges in the energy range of experimental data available.

Theory

Photoionization cross section is given by

$$\sigma = \frac{4\pi}{3}\,\omega \left|D_{if}\right|^{2} \delta(E_i - E_f - E)$$

for non-polarized isotropic radiation, where

$$D_{if} = \langle \Psi_f | D | \Psi_i \rangle$$

is the matrix element of dipole operator D

In the dipole approximation, the angular distribution is given by

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi}\left[1 + \beta P_2(\cos(\vartheta))\right]$$

where β is the photoelectron asymmetry parameter.

In the R-matrix method, photoinization cross sections are calculated using wavefunction expansions of the form as follows:

$$\Psi = A\sum_{i} \psi_i \theta_i + \sum_{j} \phi_j c_j$$

where ψ_i is the wavefunction for an N-electron system, θ_i a function for an added electron, A an operator for anti-symmetrization and vector coupling, ϕ_j a wave function for the (N+1)-electron system and c_j are coefficients to be determined. The functions ψ_i are referred to as target states. The orbitals θ_i are taken to be orthogonal to all orbitals in the ψ_i, and this constraint provides the main reason for including the functions ϕ_j. The orbitals θ_i and coefficients c_j are optimized using the R-matrix method. In the relativistic R-matrix (RR-matrix), Breit-Pauli Hamiltonian has been employed.

The wave functions used in this work are represented by expansions of the form:

$$\Psi(LS) = \Sigma\, a_i\, \Phi_i(\alpha_i LS)$$

The radial functions of the orbitals are expressed in the analytic form:

$$P_{nl}(r) = \Sigma\, C_j\, r^{P_j}\, e^{-\xi_j r}$$

Results and discussion

In the present work, the photon impact integral ionization cross section (σ) as well as photoelectron asymmetry parameter (β) for the reactions $h\nu+Ne(1s^2\,2s^2\,2p^6) \rightarrow Ne^+(1s^2\,2s^2\,2p^5) + e^-$, $h\nu+Ar(1s^2\,2s^2\,2p^6\,3s^2\,3p^6) \rightarrow Ar^+(1s^2\,2s^2\,2p^6\,3s^2\,3p^5) + e^-$, $h\nu+Kr(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^6) \rightarrow Kr^+(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^5) + e^-$ and $h\nu+Xe(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^6\,4d^{10}\,5s^2\,5p^6) \rightarrow Xe^+(1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,3d^{10}\,4s^2\,4p^6\,4d^{10}\,5s^2\,5p^5) + e^-$ have been calculated in the L-S and j-j coupling schemes using Hartree-Fock (HF) wavefunctions within the reliable non-relativistic R-matrix as well as relativistic R-matrix (RR-matrix) methods in both the length and velocity gauges in the energy range of experimental data available. Comparison is made with all available experimental data as well as other theoretical results.

Figure 1 exhibits our present R-matrix total photoionization cross sections of neon atomic system along with other experimental as well as theoretical results from the threshold to about 400 eV energy range. It is clear from this figure that our R-matrix results in both length and velocity gauges are in good agreement with other theoretical predictions and experimental sections which show that the effect of relativity and correlation is negligible in this case.

Figure 2 displays our R-matrix integral photoionization cross sections of argon (Ar) atomic system along with other available theoretical and experimental results. It is seen from this figure that in the low energy range, the length form is better than the velocity form of cross sections which indicates that the length gauge is valid in the low energy region and the velocity form is good in the intermediate energy range. However, there is considerable disagreement between our results and experimental data, which shows the importance of correlation and relativity.

Figure 3 gives the photoelectron asymmetry parameter for the argon 3p ionization. It is clear from this figure that in the low energy range, there is a reasonably good agreement between our present results and other results but in the vicinity of the minimum, there is a discrepancy.

Figure 4 presents the total photoionization cross sections of the krypton (Kr) atomic system along with other available experimental observations as well as theoretical predictions. It is clear from this figure that the length form is better than the velocity form in the low energy region as in the other cases of Ne and Ar. There are some structures in the ionization cross sections which are probably due to excitation of other subshells. Figure 5 gives the photoelectron asymmetry parameter for the krypton 4p ionization. There is considerable disagreement among our present results and other results which indicates the importance of correlation, relativity, interchannel interaction as well as intrachannel interaction.

Figure 6 exhibits the integral photoionization cross section curves for the xenon (Xe) atomic system in the length and velocity gauges with other available experimental observations and theoretical predictions. It is clear from this figure that the effect of relativity is considerable. There are some structures in the ionization curves which are probably due to excitation of other subshells. In the vicinity of maximum, our present approach completely breaks down which clearly shows that the independent particle model (IPM) is not good in this situation. Figure 7 gives the photoelectron asymmetry parameter for the xenon 5p ionization. In this case the situation is very discouraging. It is crystal clear that IPM completely breaks down in the case of the heaviest noble gas atom xenon. It is indispensable to include the effect of (1) correlation, (2) relativity, (3) intrachannel interaction and (4) interchannel interaction in order to obtain high precision results.

Conclusion and future direction

Our present theoretical investigation clearly demonstrates that the effect of correlation and relativity in the case of lighter noble gas atom neon is negligible. These effects increase with the increase of atomic number (Z). In the case of the heavy rare gas atom xenon, there is a complete breakdown of independent particle approximation which demonstrates the importance of correlation and relativity. HF cross sections are both qualitatively as well as quantitatively incorrect in the entire energy range which exhibit that the multielectron correlation as well as relativity are both important but interchannel interactions are more important than the intrachannel interaction and relativity for obtaining high precision results.

Our present results suggest that full configuration interaction wave functions must be used in the R-matrix as well as RR-matrix in order to obtain high precision results. The output of CIV3, SS, MCHF, Cowan, and MCDF may be input to the R-matrix and RR-matrix for accurate predictions.

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FIGURE CAPTIONS

Figure 1 Total photon impact ionization cross section (σ) for the 2p-subshell of neon.
Present R-matrix results in length form
Present R-matrix results in velocity form
Wulleumier (Ref.228)
Saito (Ref.228)
Marr (Ref.228)
Wulleumier (Ref.228)
Berkowitz (Ref.228)
Yeh (Ref.228)
Johnson (Ref.228)
Kennedy (Ref.228)

Figure 2 Total photon impact ionization cross section (σ) for the 3p-subshell of argon.
Present R-matrix results
Langer (Ref.228)
Chan (Ref.228)
Adam (Ref.228)
Barkowitz (Ref.228)
Tulkki (Ref.228)
Wijesundera (Ref.228)
Huang (Ref.228)

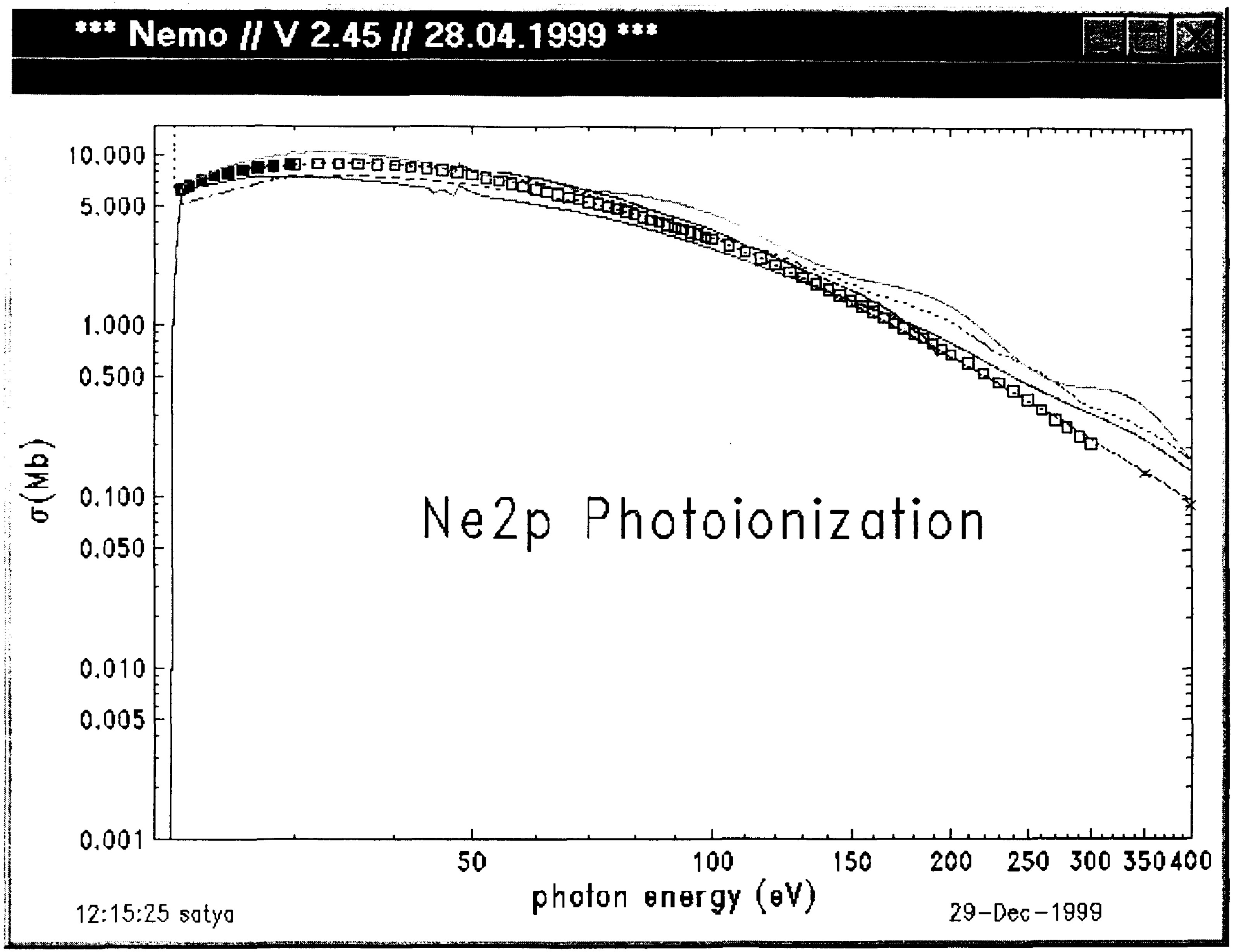
Figure 3 Photoelectron asymmetry parameter (β) for argon.
Present R-matrix results
Langer (Ref.228)
Southworth (Ref.228)
Adam (Ref.228)
Dahmer (Ref.228)
Houlgate (Ref.228)
Tulkki (Ref.228)
Wijesundera. (Ref.228)
Huang (Ref.228)
Amusia (Ref.228)

Figure 4 Total photon impact ionization cross section (σ) for the 4p-subshell of krypton.
Present R-matrix results
Berrah (Ref.228)
Tulkki (Ref.228)
Aksela (Ref.228)
Samson (Ref.228)
Berkowitz (Ref.228)
Tulkki (Ref.228)
Huang (Ref.228)

Figure 5 Photoelectron asymmetry parameter (β) for krypton.
Present R-matrix results
Berrah (Ref.228)
Southworth (Ref.228)
Miller (Ref.228)
Dahmer (Ref.228)
Yah (Ref.228)
Tulkki (Ref.228)
Huang (Ref.228)

Figure 6 Total photon impact ionization cross section (σ) for the 5p-subshell of xenon.
Present R-matrix results
Present RR-matrix results
Becker (Ref.228)
Fahlmann (Ref.228)
Adam (Ref.228)
Berkowitz ((Ref.228)
Kutzner (Ref.228)

Figure 7 Photoelectron asymmetry parameter (β) for xenon.
Present R-matrix results
Southworth (Ref.228)
Southworth (Ref.228)
Krause (Ref.228)
Torop (Ref.228)
Dahmer (Ref.228)
Kutzner (Ref.228)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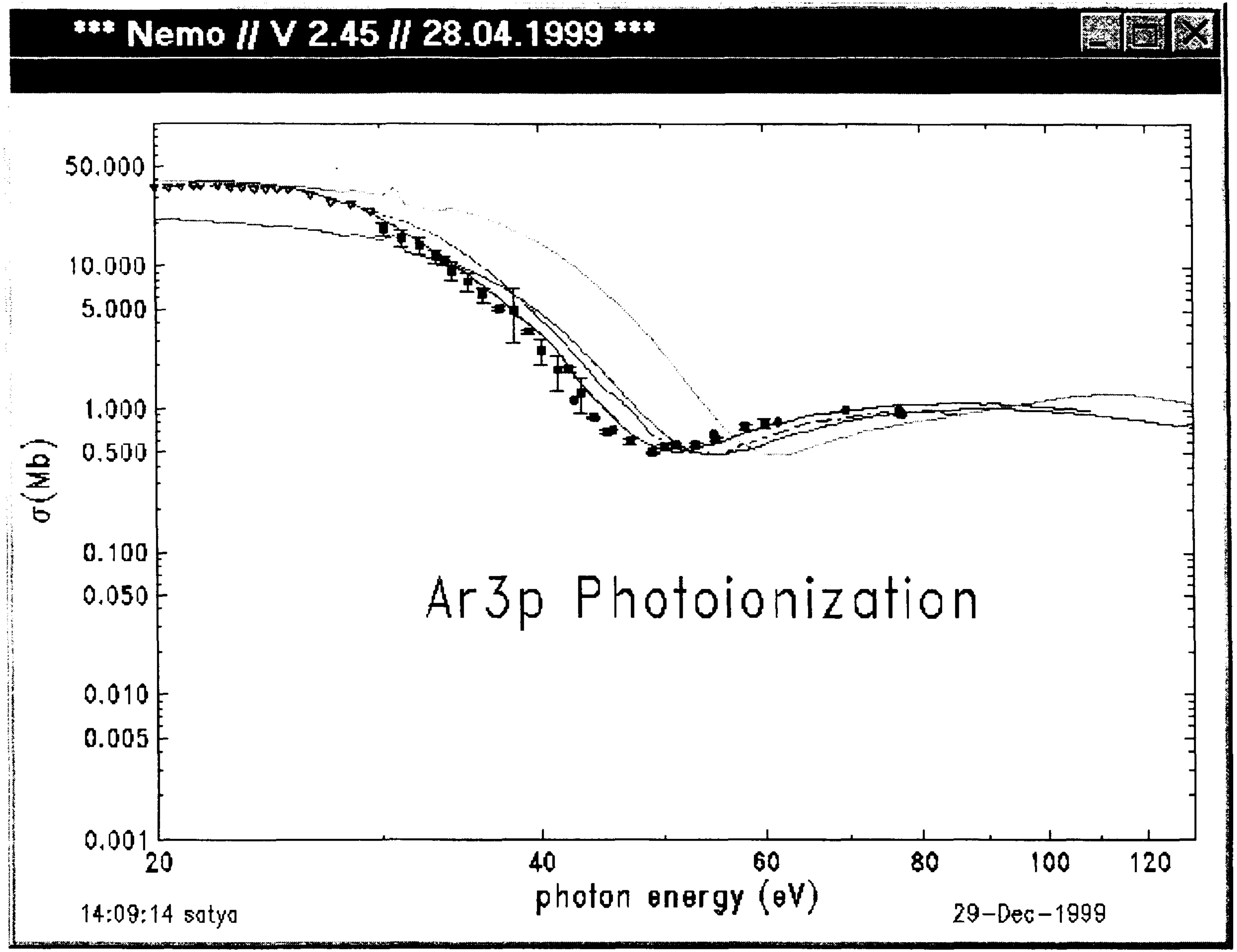
σ(Mb)
10.000
5.000
1.000
0.500
0.100
0.050
0.010
0.005
0.001
50
100
150
200
250
300
350
400
photon energy (eV)
Ne2p Photoionization
12:15:25 satya
29-Dec-1999

Fig.1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Ar3p Photoionization
σ(Mb)
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10.000
5.000
1.000
0.500
0.100
0.050
0.010
0.005
0.001
20
40
60
80
100
120
photon energy (eV)
14:09:14 satya
29-Dec-1999

Fig.2

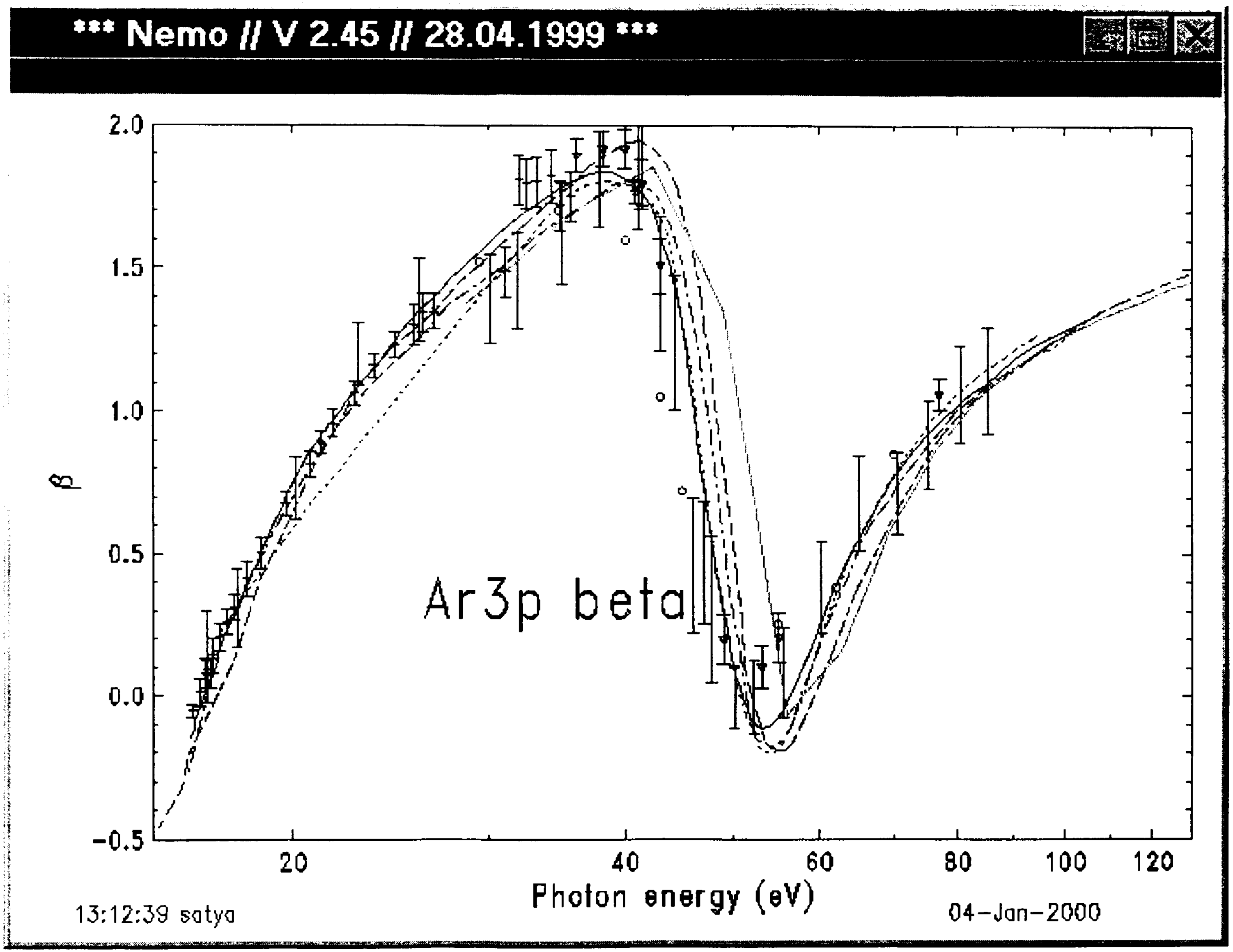
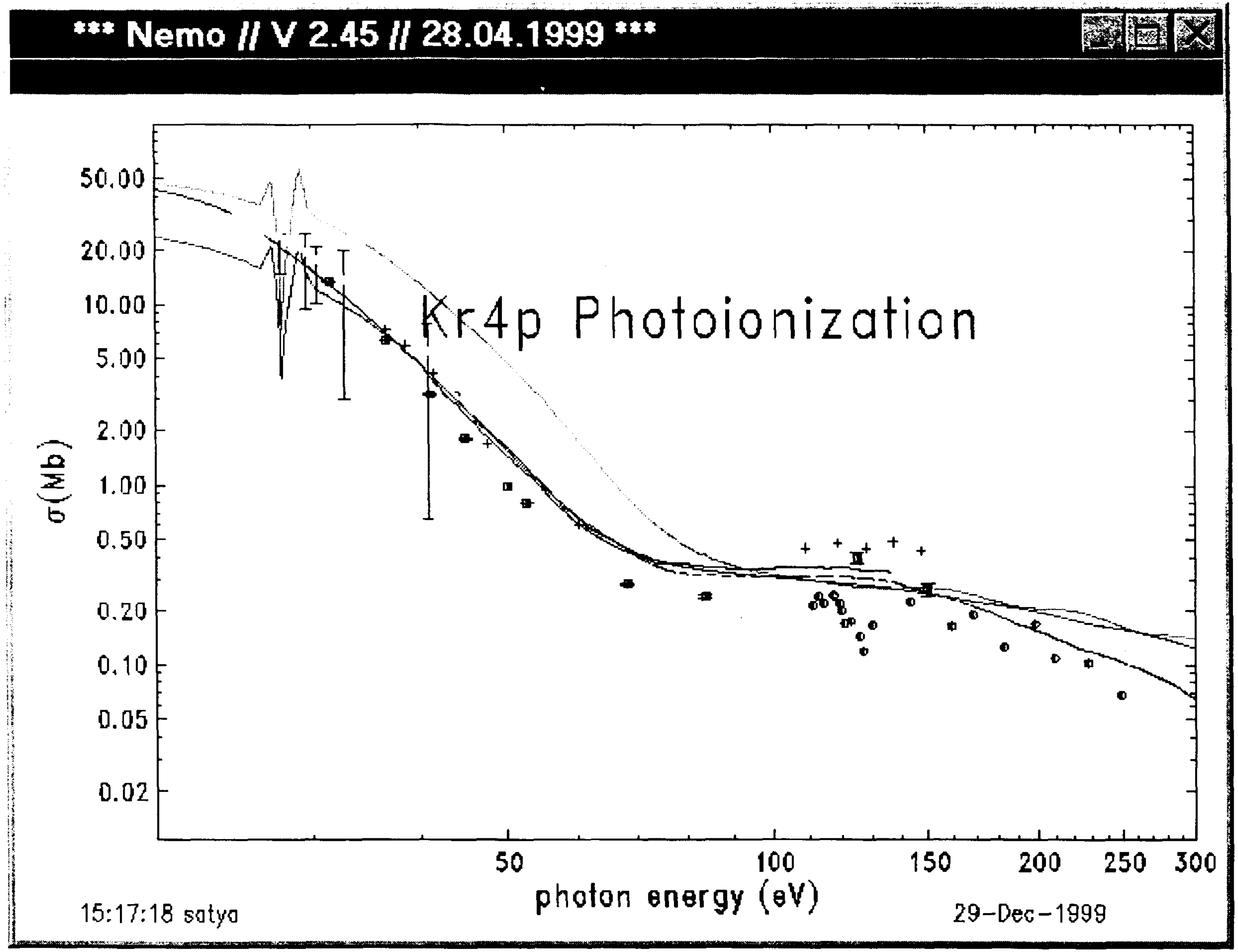

*** Nemo // V 2.45 // 28.04.1999 ***
2.0
1.5
1.0
0.5
0.0
−0.5
β
Ar3p beta
20
40
60
80
100
120
Photon energy (eV)
13:12:39 satya
04-Jan-2000

Fig.3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Kr4p Photoionization
σ(Mb)
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20.00
10.00
5.00
2.00
1.00
0.50
0.20
0.10
0.05
0.02
50
100
150
200
250
300
photon energy (eV)
15:17:18 satya
29-Dec-1999

Fig.4

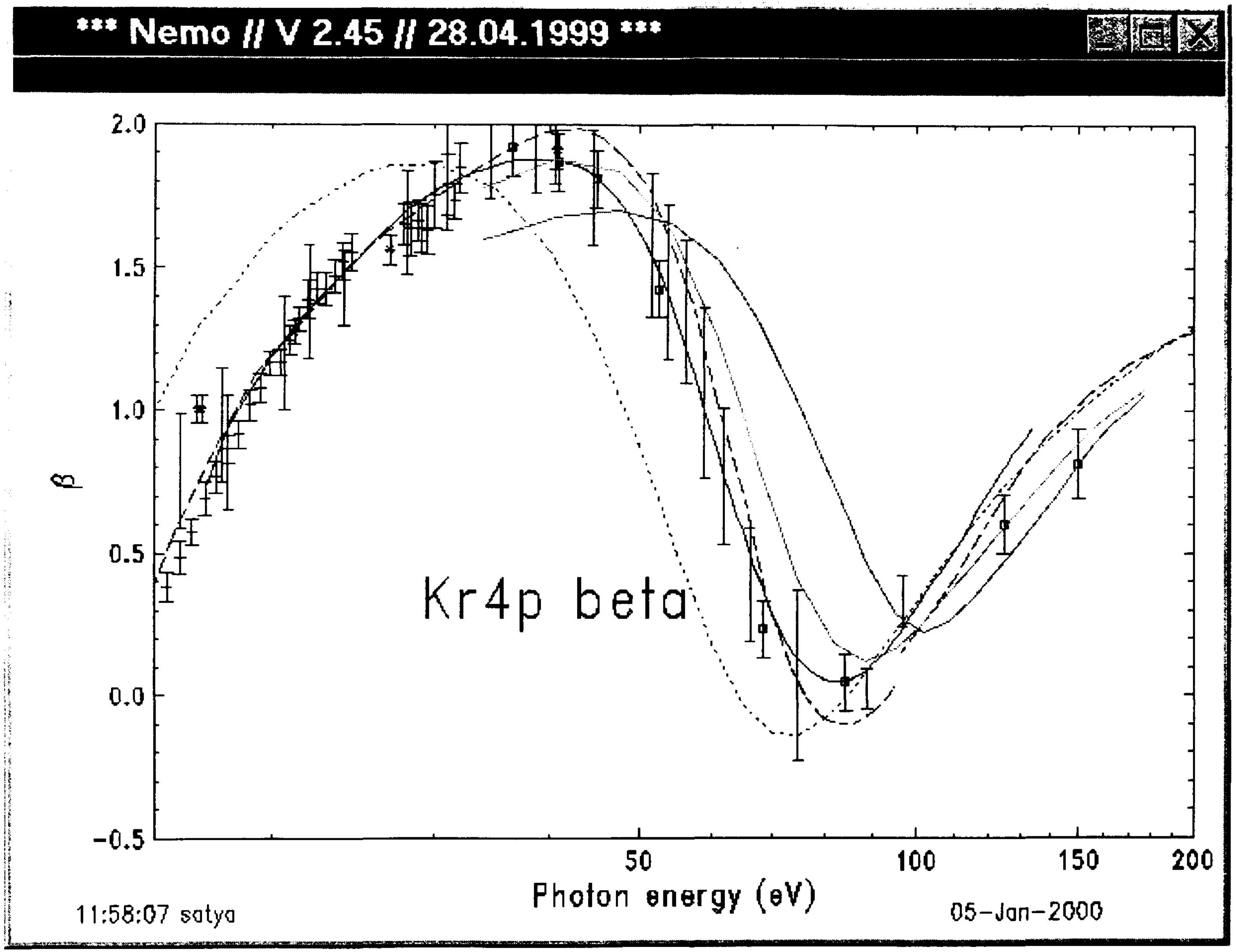
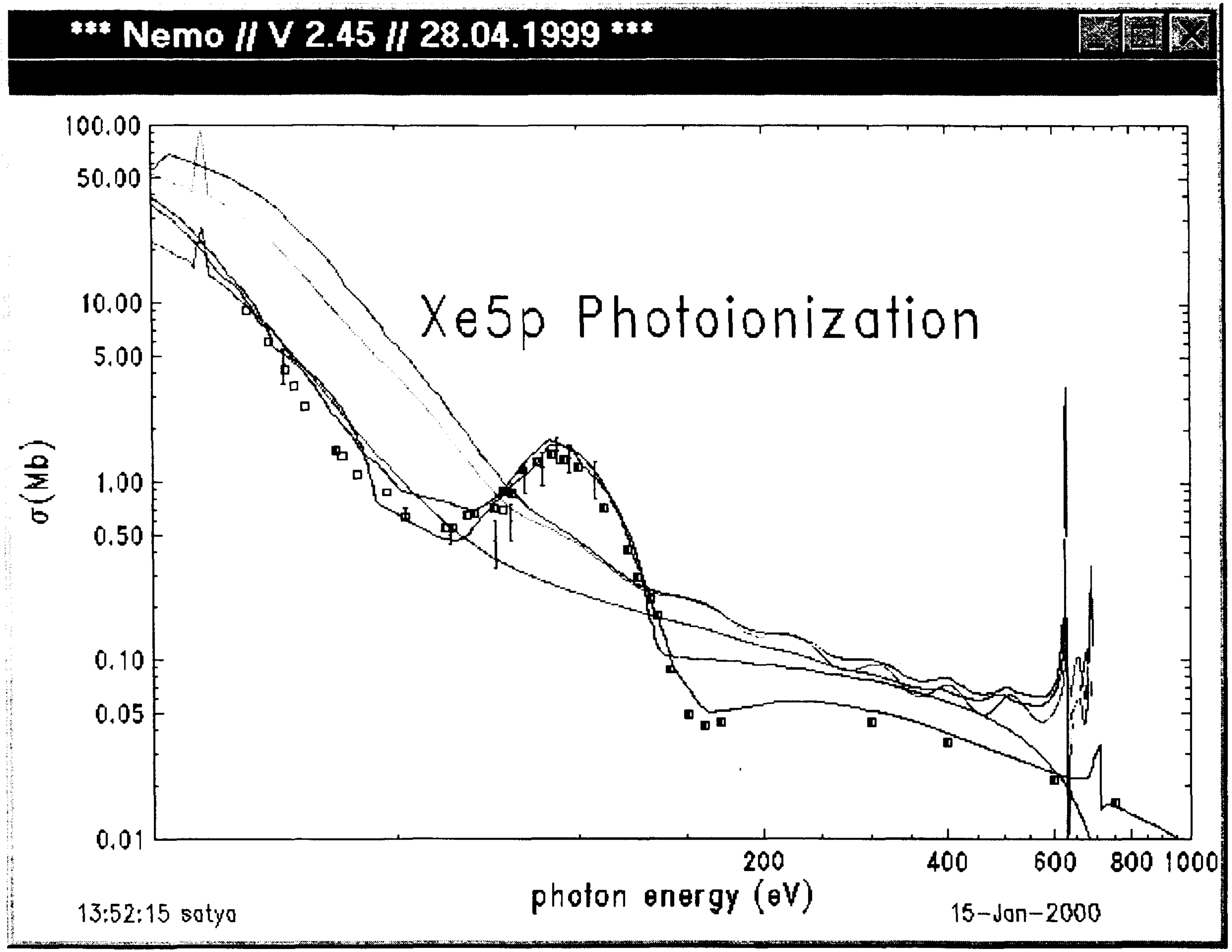

*** Nemo // V 2.45 // 28.04.1999 ***
Kr4p beta
β
2.0
1.5
1.0
0.5
0.0
−0.5
50
100
150
200
Photon energy (eV)
11:58:07 satya
05-Jan-2000

Fig.5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Xe5p Photoionization
σ(Mb)
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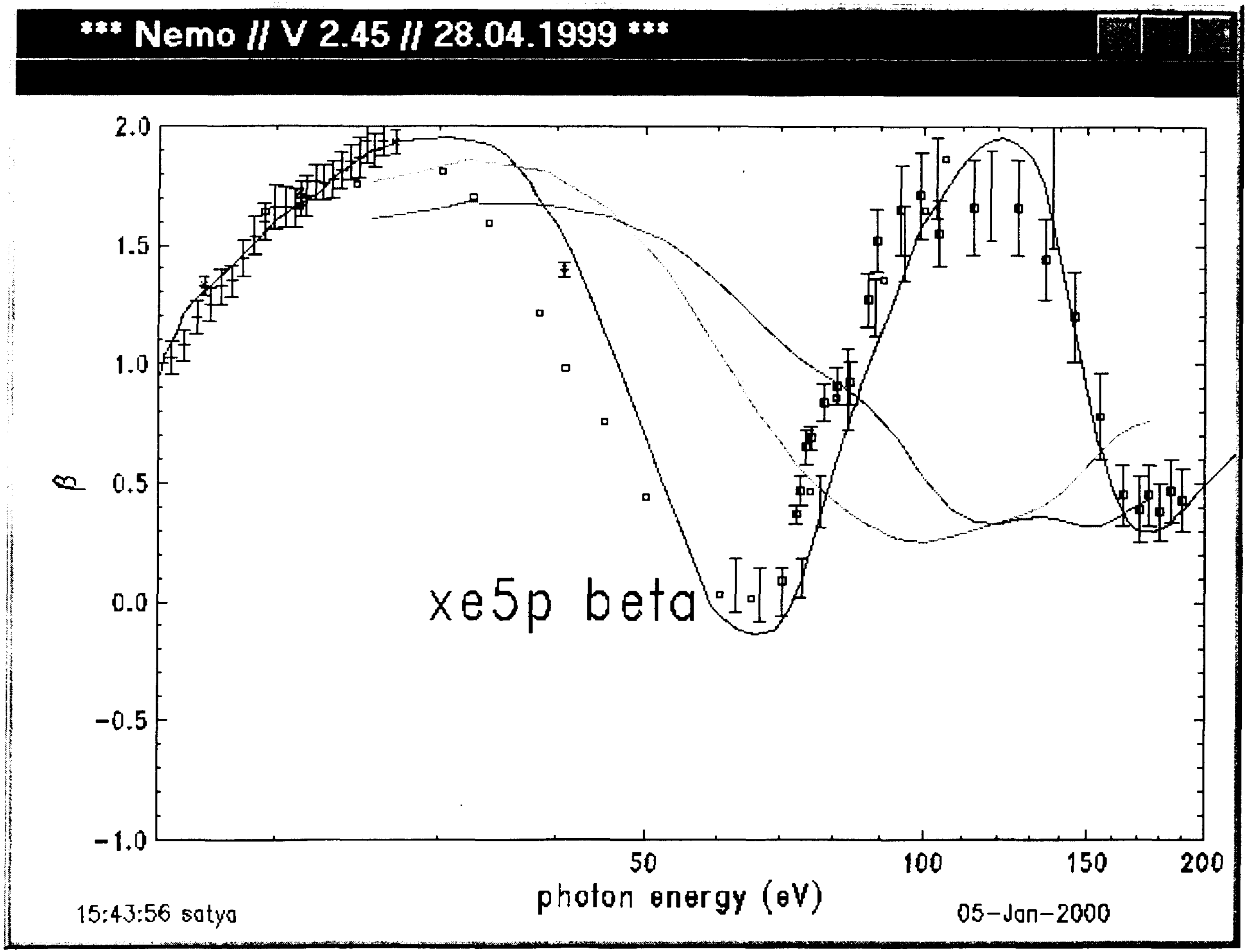
50.00
10.00
5.00
1.00
0.50
0.10
0.05
0.01
200
400
600
800
1000
photon energy (eV)
13:52:15 satya
15-Jan-2000

Fig.6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2.0
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1.0
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0.0
−0.5
−1.0
β
xe5p beta
50
100
150
200
photon energy (eV)
15:43:56 satya
05−Jan−2000

Fig.7