T3191 JS ②

PREPARED FOR THE U.S. DEPARTMENT OF ENERGY,
UNDER CONTRACT DE-AC02-76-CHO-3073

PPL-2796
JC-426

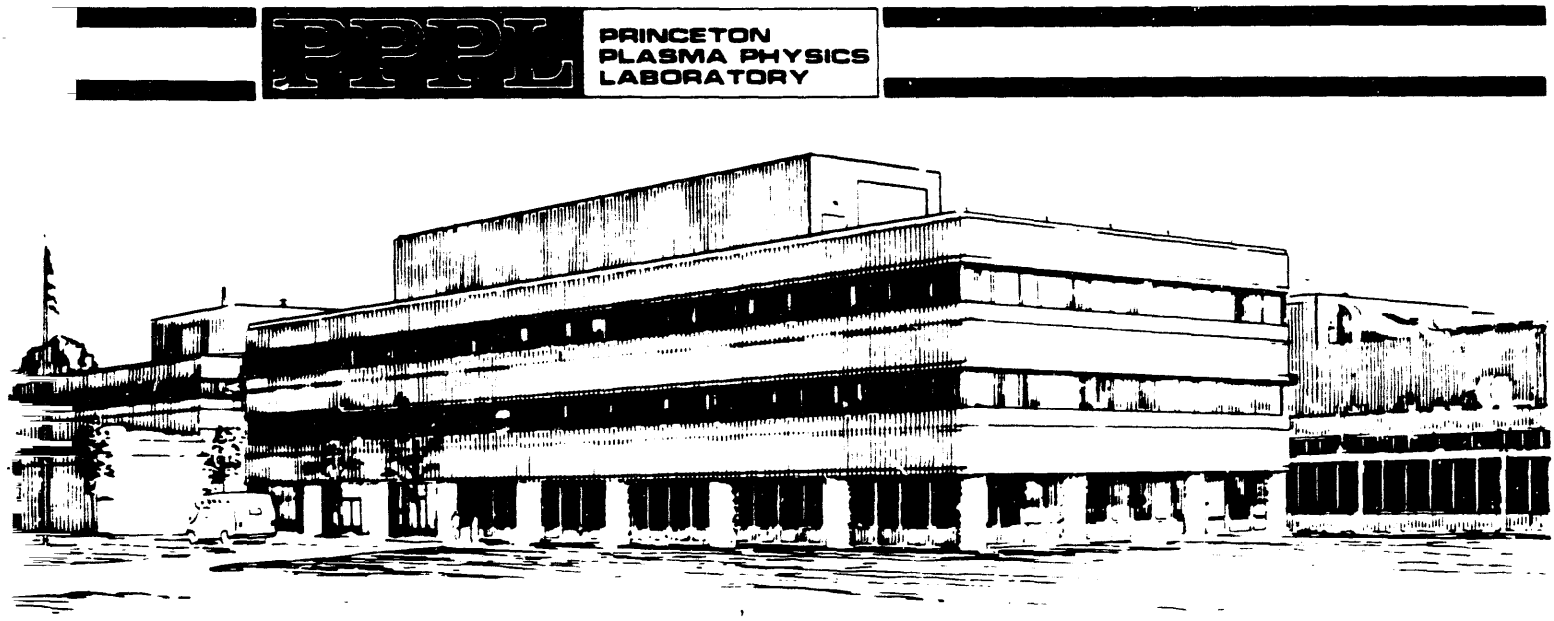
PPPL-2796

COMPARISON OF EXPLICIT CALCULATIONS FOR $n = 3$ TO 8 DIELECTRONIC SATELLITES OF THE FeXXV Kα RESONANCE LINE WITH EXPERIMENTAL DATA FROM THE TOKAMAK FUSION TEST REACTOR

BY

V. DECAUX, M. BITTER, H. HSUAN,
K.W. HILL, S. VON GOELER, H. PARK, AND C.P. BHALLA

December 1991



PRINCETON UNIVERSITY, PRINCETON, NEW JERSEY

DISTRIBUTION

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial produce, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

NOTICE

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the:

Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831;
Prices available from (615) 576-8401.

Available to the public from the:

National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22161
703-487-4650

PPPL--2796

DE92 003994

Comparison of explicit calculations for $n = 3$ to 8 dielectronic satellites of the FeXXV Kα resonance line with experimental data from the Tokamak Fusion Test Reactor

V. Decaux,* M. Bitter, H. Hsuan, K. W. Hill, S. von Goeler, and H. Park
Princeton Plasma Physics Laboratory, Princeton University, Princeton, New Jersey 08543

C. P. Bhalla
Department of Physics, Kansas State University, Manhattan, Kansas 66506

ABSTRACT

Dielectronic satellite spectra of the FeXXV Kα resonance line observed from the Tokamak Fusion Test Reactor (TFTR) plasmas have been compared with recent explicit calculations for the n = 3 to 8 dielectronic satellites as well as the earlier theoretical predictions, which were based on the $1/n^3$ scaling law for $n > 4$ satellites. The analysis has been performed by least-squares fits of synthetic spectra to the experimental data. The synthetic spectra constructed from both theories are in good agreement with the observed data. However, the electron temperature values obtained from the fit of the present explicit calculations are in better agreement with independent measurements.

---

* Permanent address: *Laboratoire de Physique Atomique et Nucléaire - Institut du Radium, Université Pierre et Marie Curie, F-75231 Paris Cedex 05, France.*

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

It is well known[1-5] that the Kα resonance line of heliumlike ions is blended with lithiumlike dielectronic satellites due to transitions $1s^2\,nl$ - $1s2p\,nl$ with $n \geq 3$. These unresolved satellites lead to a significant increase in both the apparent width and intensity of the resonance line, which must be taken into account for Doppler broadening and Doppler shift measurements, as well as the evaluation of satellite to resonance line ratios, which are used for diagnostics of solar flares and tokamak plasmas.[5-10] In view of these important diagnostic applications, it is necessary to determine the contribution of these satellites as well as possible. However, explicit calculations of the high-n satellite line strengths are difficult, due to the fact that the number of intermediate resonance states increases rapidly with the principal quantum number n of the outermost occupied shell of the resonance state. As a result, explicit calculations[1,11-15] have been limited so far to low-lying resonance states with $n \leq 4$, while an approximate $1/n^3$ scaling law has generally been used to extrapolate the satellite intensity factors for $n > 4$.

In order to test the validity of this approximation, Karim and Bhalla have recently performed explicit calculations of n = 3 to 8 dielectronic satellite line strengths using the Hartree-Fock atomic model for NeVII, SiXIII, ArXVII, TiXXI, CrXXIII, and NiXXVII.[16] They found that the n-threshold above which the $1/n^3$ scaling law provides good approximation varies with Z. For high-Z ions, the $1/n^3$ scaling law can be applied if $n \geq 5$, whereas for low-Z ions ($Z \leq 14$) it can only be applied if $n \geq 8$. The purpose of this paper is to compare recent explicit Hartree-Fock model calculations for the n = 3 to 8 dielectronic satellites of FeXXV and the earlier theoretical results from Bely-Dubau *et al.*,[1] who used the $1/n^3$ scaling law for dielectronic satellites with $n > 4$, with experimental spectra.

The experimental data were recorded from ohmically-heated TFTR plasmas with a central major radius R = 2.70 m and minor radius a = 0.95 m, which were fueled by the injection of solid deuterium pellets. There was also a small amount of radio-frequency heating (0.5, 0.6, and 1.0 MW, respectively, for each of the three discharges we analyzed) from 3.3 to 3.8 s. Pellet injections result in large electron density increases, as shown in Fig. 1, which are correlated with a sudden drop of the electron temperature. As a result, pellet injections in ohmically-heated discharges provide ideal experimental conditions for the study of high-n dielectronic satellites, which are then very pronounced due to the facts that (1) the intensities of the dielectronic satellites relative to the resonance line increase with decreasing electron temperatures, and (2) the Doppler broadening of the lines is substantially reduced since the ion temperatures T_i are low ($T_i \approx T_e$), so that a large fraction of the n = 3 satellites is resolved from the resonance line.

Figure 2 presents spectra obtained after the injection of the second pellet during the period from 4.5 to 5.0 s from the TFTR high-resolution vertical X-ray crystal spectrometer[17] at a plasma major radius R = 2.41 m. The data have been accumulated from three very similar discharges in order to reduce the statistical errors. Since most of the $n \geq 3$ dielectronic satellites are blended with the Kα resonance line, we performed a least-squares fit of synthetic spectra constructed from the present calculations [Fig. 2(a)] and from the theory of Bely-Dubau *et al.*[1] [Fig. 2(b)] to the experimental data. The results from both fits, which include the individual contributions from the different n shells, are shown in Fig. 2 by solid lines. The present calculations were performed using the Hartree-Fock atomic model for the following cases: 1s2pnp (n = 2 - 8), 1s2pns (n = 2 - 8), 1s2pnd (n = 3 - 8), 1s2pnf (n = 4 - 8), and 1s2snp (n = 2 - 8); the details of the calculations are given in Ref. 16. On the other hand, the calculations of Bely-Dubau *et al.*[1] are based on the scaled Thomas-Fermi atomic model and used the $1/n^3$ scaling law for dielectronic

satellites with n = 5 to 16. The synthetic spectrum from the present explicit calculations shown in Fig. 2(a) is composed of approximately 100 spectral lines. Since these calculations have only been carried out up to n = 8, we have taken the extrapolated data of Bely-Dubau *et al.*[1] only up to n = 8 in order to make a sensible comparison of the two theories. Since the spectrometer has no absolute wavelength calibration, the experimental wavelengths have been normalized to the value of 1.85026 Å for the Kα resonance line obtained by Briand *et al.* from an absolute wavelength measurement in beam-foil experiments.[18] Similarly, the theoretical wavelengths from the present calculations have been shifted by a constant amount of 1.86 mÅ, and the wavelengths from Bely-Dubau *et al.*[1] were shifted by 0.36 mÅ.

The least-squares fits allowed us to determine best values for the electron temperatures, upon which the ratios of the dielectronic satellites to resonance line intensity solely depend.[1,19] The T_e results from these fits have been compared with the values provided by independent measurements from the TFTR Pulse Height Analysis (PHA) system,[20] and are shown in Fig. 3 for five time intervals of 500 ms ranging from 3.5 to 6.0 s. The PHA values shown in Fig. 3 were obtained from an interpolaticn of results measured at R = 2.08 m and R = 2.70 m, using radial profiles of the electron cyclotron emission which was measured by the TFTR radiometer. The estimated errors for these PHA results are typically of the order of 10%. The error bars for the T_e values obtained from the least-squares fits were typically of the order of 50 eV. These error bars reflect the good agreement between the synthetic and observed spectra, since the statistical errors of the experimental data were small.

The T_e values obtained from the fit of the present explicit calculations are in better agreement with the PHA results than the ones obtained from the fit of the data of Bely-Dubau *et al.*[1] using the $1/n^3$ scaling law. The difference of typically 200 eV in the electron temperature results obtained from the two theories cannot be ascribed to differences in the theoretical predictions for the satellite to resonance line intensity ratios, which are in fact very similar for both theories, as shown in Fig. 4: this confirms previous findings from Karim and Bhalla[16] that the $1/n^3$ scaling law should be applicable for iron. We assume that the difference in the T_e values obtained from both theories can be explained by small differences in the predicted wavelengths. We note that in the calculation of Bely-Dubau *et al.*,[1] the wavelengths for the dielectronic satellites from each n shell with $n \geq 5$ were grouped under a unique value, which was also determined by a scaling law, while the wavelengths were explicitly calculated for each line in the present paper.

ACKNOWLEDGMENTS

We gratefully acknowledge the continuing support of Dr. K. M. Young, and the technical assistance of J. Gorman, R. Such, and the TFTR operating crew. We also thank N. Schechtman for developing software for the data analysis. This work was supported by the U.S. Department of Energy (DOE), Contract No. DE-AC02-76-CHO-3073. One of us (C.P.B.) was supported by the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research, U.S. DOE.

References

[1] F. Bely-Dubau, A. H. Gabriel, and S. Volonté, Mon. Not. R. Astron. Soc. **189**, 801 (1979).

[2] J. Dubau, A. H. Gabriel, M. Loulergue, L. Steenman-Clark, and S. Volonté, Mon. Not. R. Astron. Soc. **195**, 705 (1981).

[3] F. Bely-Dubau, P. Faucher, L. Steenman-Clark, M. Bitter, S. von Goeler, K. W. Hill, C. Camhy-Val, and J. Dubau, Phys. Rev. A **26**, 3549 (1982).

[4] M. Bitter, K. W. Hill, M. Zarnstorff, S. von Goeler, R. Hulse, L. C. Johnson, N. R. Sauthoff, S. Sesnic, K. M. Young, M. Tavernier, F. Bely-Dubau, P. Faucher, M. Cornille, and J. Dubau, Phys. Rev. A **32**, 3011 (1985).

[5] M. Bitter, S. von Goeler, K. W. Hill, R. Horton, D. Johnson, W. Roney, N. R. Sauthoff, E. Silver, and W. Stodiek, Phys. Rev. Lett. **47**, 921 (1981).

[6] M. Bitter, K. W. Hill, N. R. Sauthoff, P. C. Efthimion, E. Meservey, W. Roney, S. von Goeler, R. Horton, M. Goldman, and W. Stodiek, Phys. Rev. Lett. **43**, 129 (1979).

[7] Y. I. Grineva, V. I. Karov, V. V. Korneev, V. V. Krutov, S. L. Mandelstam, L. A. Vainshtein, B. N. Vasilysev, and J. A. Zhitnik, Sol. Phys. **29**, 441 (1973).

[8] K. Tanaka, T. Watanabe, K. Nishi, and K. Akita, Astrophys. J., **254**, L59 (1982).

[9] U. Feldman, G. A. Doschek, and R. W. Kreplin, Astrophys. J., **238**, 365 (1980).

[10] J. L. Culhane, A. H. Gabriel, L. W. Acton, C. G. Rapley, K. J. Phillips, C. J. Wolfson, E. Antonucci, R. D. Bentley, R. C. Catura, C. Jordan, M. A. Kayat, B. J. Kent, J. W. Leibacher, A. N. Parmar, J. C. Sherman, L. A. Springer, K. T. Strong, and N. J. Veck, Astrophys. J. **244**, L141 (1981).

[11] J. Nilsen, At. Data Nucl. Data Tables **37**, 191 (1987); **38**, 339 (1988).

[12] M. H. Chen, At. Data Nucl. Data Tables **34**, 101 (1986); Phys. Rev. A **38**, 3280 (1988).

[13] F. Bombarda, R. Giannella, E. Källne, G. J. Tallents, F. Bely-Dubau, P. Faucher, M. Cornille, J. Dubau, and A. H. Gabriel, Phys. Rev. A **37**, 504 (1988).

[14] C. P. Bhalla and K. R. Karim, Phys. Rev. A **34**, 3525 (1986); C. P. Bhalla, K. R. Karim, and T. Reeves, Phys. Scr. **34**, 747 (1986).

[15] F. Bely-Dubau, A. H. Gabriel, and S. Volonté, Mon. Not. R. Astron. Soc. **186**, 405 (1979).

[16] K. R. Karim and C. P. Bhalla, Phys. Rev. A **43**, 615 (1991).

[17] M. Bitter, K. W. Hill, S. Cohen, S. von Goeler, H. Hsuan, L. C. Johnson, R. Raftopoulos, M. Reale, N. Schechtman, S. Sesnic, F. Spinos, J. Timberlake, S. Weicher, N. Young, and K. M. Young, Rev. Sci. Instrum. **57**, 2145 (1986).

[18] J. P. Briand, M. Tavernier, R. Marrus, and J. P. Desclaux, Phys. Rev. A **29**, 3143 (1984).

[19] A. H. Gabriel, Mon. Not. R. Astron. Soc. **160**, 99 (1972).

[20] K. W. Hill, M. Bitter, M. Diesso, L. Dudek, S. von Goeler, S. Hayes, L. C. Johnson, J. Kiraly, E. Moshey, G. Renda, S. Sesnic, N. R. Sauthoff, F. Tenney, and K. M. Young, Rev. Sci. Instrum. **56**, 840 (1985).

FIGURE CAPTIONS

Fig. 1 Line-averaged electron density as a function of time from a TFTR discharge with injection of solid deuterium pellets at 2 and 3 s. The data were measured with the TFTR infrared interferometer at a plasma major radius R = 2.47 m. The plasma center was at R = 2.70 m, as determined by the magnetic axis.

Fig. 2 Spectrum of the FeXXV Kα resonance line accumulated from three very similar TFTR discharges during the period from 4.5 to 5.0 s after the injection of the second pellet (circles). The solid lines represent least-squares fits of synthetic spectra constructed from (a) present calculations and (b) the theory of Bely-Dubau *et al.* (Ref. 1) to the experimental data. Shown are the individual contributions from the resonance line and the $n = 3$, $n = 4$, and $n = 5$ to 8 satellites, as well as the sum of these components.

Fig. 3 Comparison of the electron temperature values derived from least-squares fits of the synthetic spectra constructed from the present calculations and the theory of Bely-Dubau *et al.* (Ref. 1) with the results from the PHA system.

Fig. 4 Theoretically predicted intensity ratios of the dielectronic satellites to the resonance line as a function of the electron temperature. Contributions from the $n = 3$, $n = 4$, and $n = 5$ to 8 shells are labeled (a), (b), (c), respectively, for present calculations and (a'), (b'), (c') for the theory of Bely-Dubau *et al.* (Ref. 1).

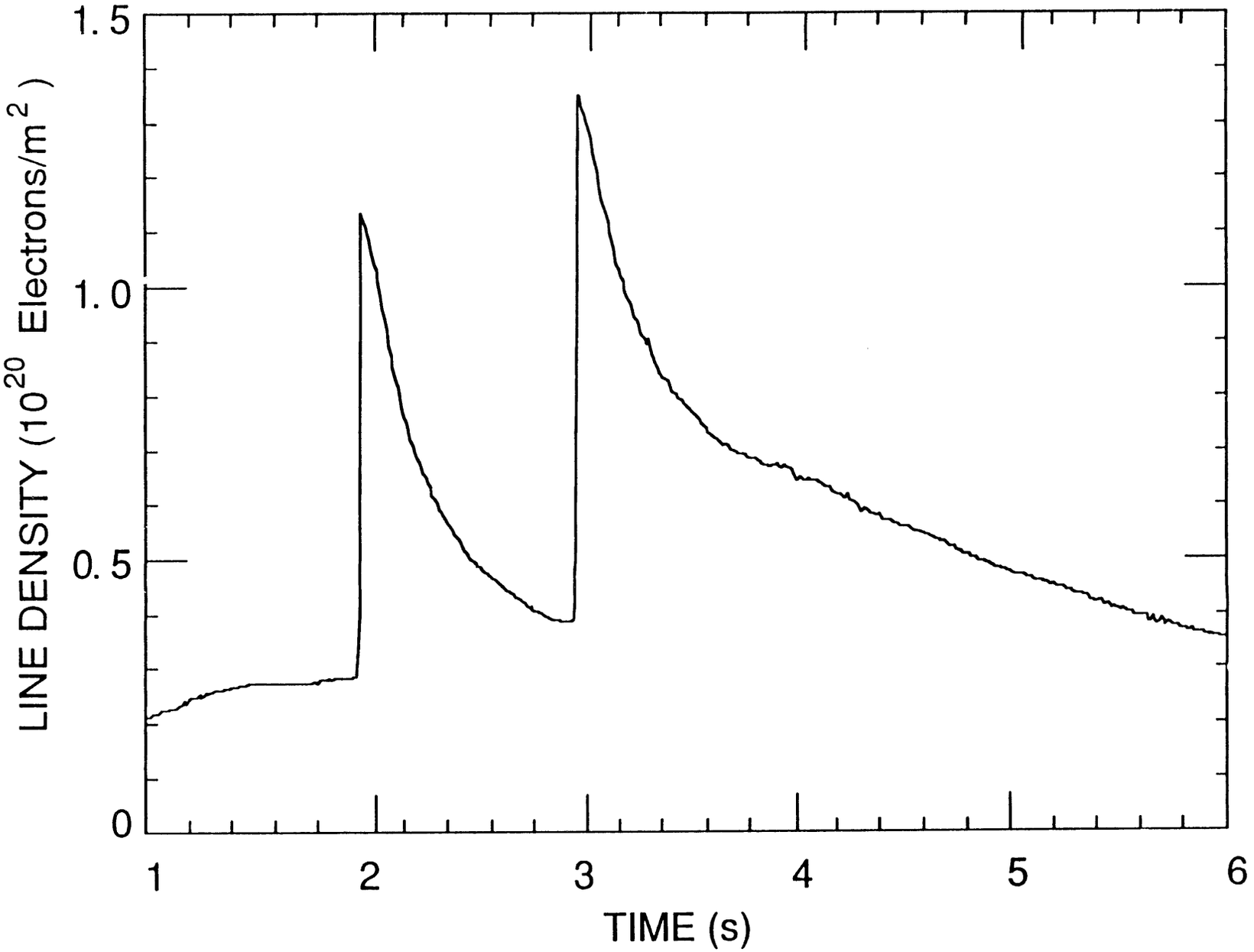


Figure 1

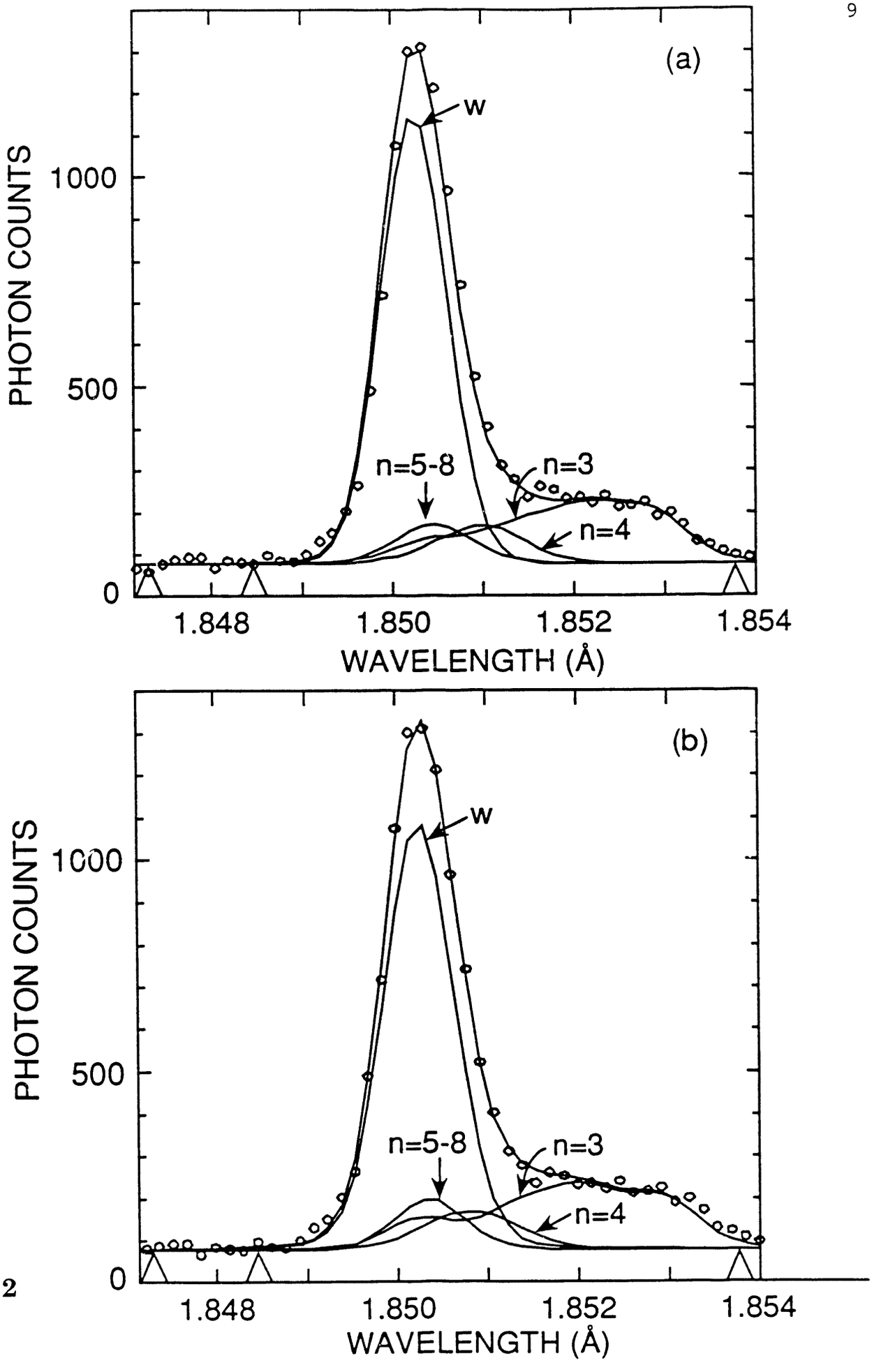

(a)
w
n=5-8
n=3
n=4
PHOTON COUNTS
1000
500
0
1.848
1.850
1.852
1.854
WAVELENGTH (Å)
(b)
w
n=5-8
n=3
n=4
PHOTON COUNTS
1000
500
0
1.848
1.850
1.852
1.854
WAVELENGTH (Å)

Figure 2

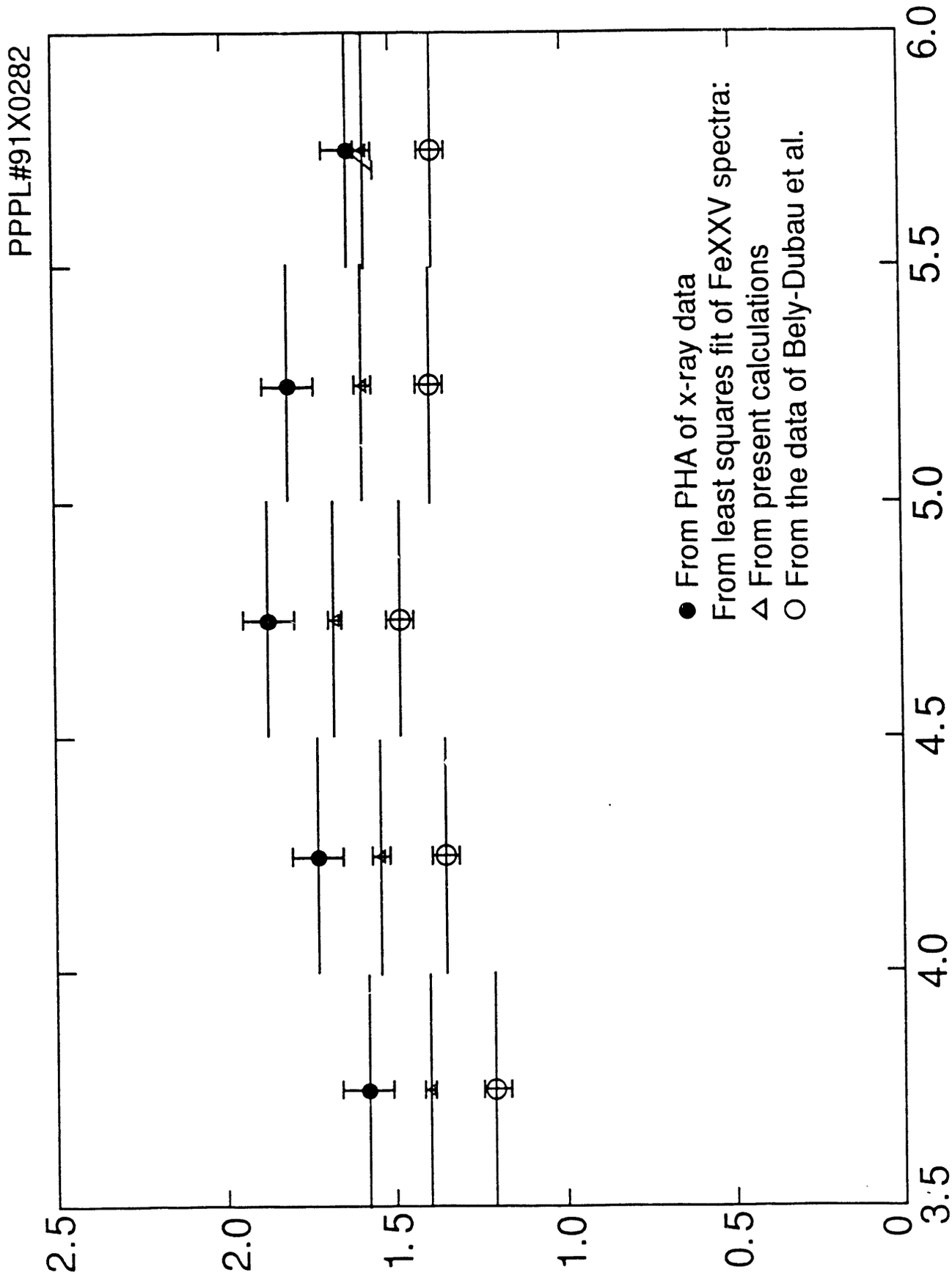

PPPL#91X0282
ELECTRON TEMPERATURE (keV)
TIME (s)
● From PHA of x-ray data
From least squares fit of FeXXV spectra:
△ From present calculations
○ From the data of Bely-Dubau et al.
2.5
2.0
1.5
1.0
0.5
0
3.5
4.0
4.5
5.0
5.5
6.0

Figure 3

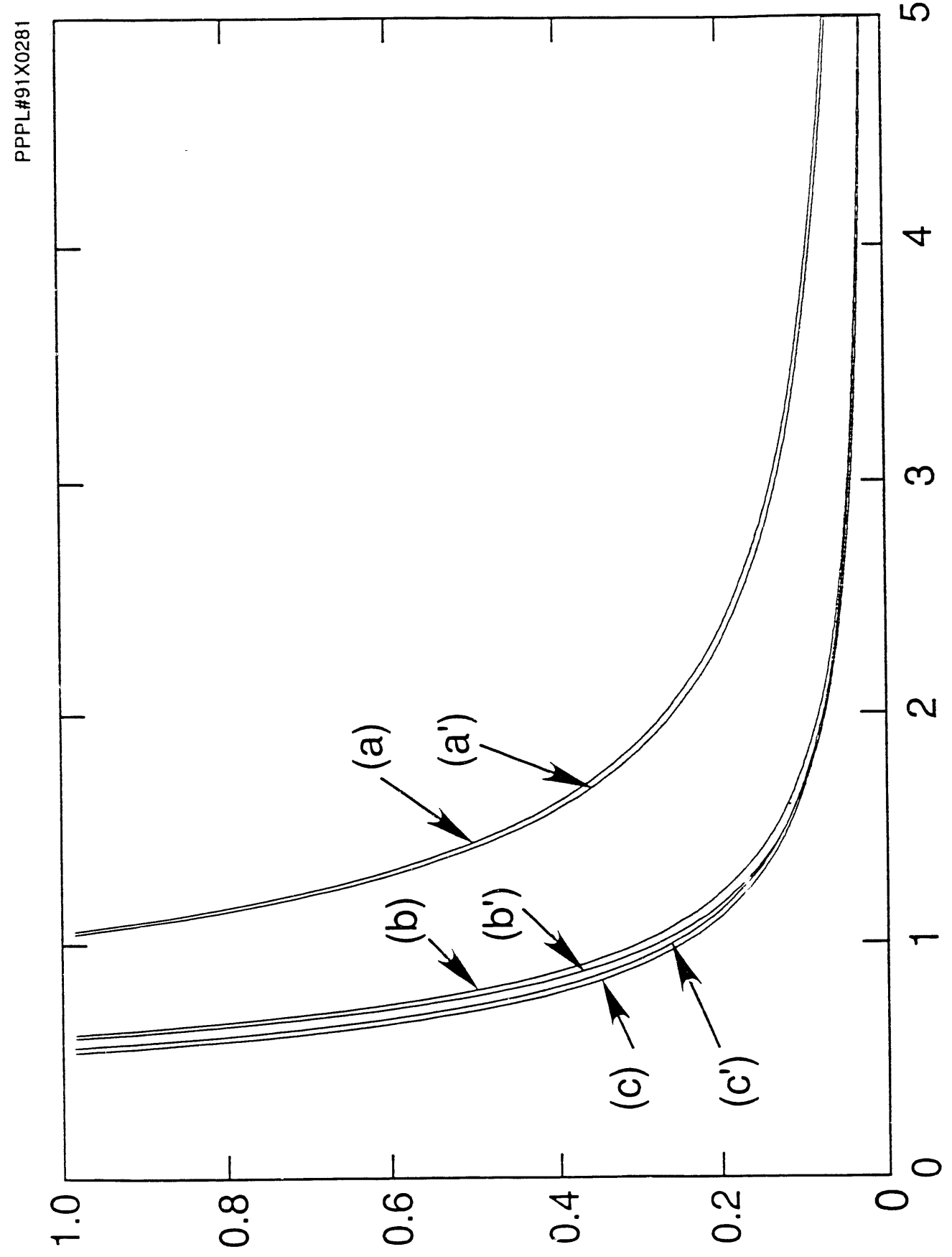

PPPL#91X0281
RELATIVE SATELLITE TO
RESONANCE LINE INTENSITIES
1.0
0.8
0.6
0.4
0.2
0
0
1
2
3
4
5
ELECTRON TEMPERATURE (keV)
(a)
(a')
(b)
(b')
(c)
(c')

Figure 4

EXTERNAL DISTRIBUTION IN ADDITION TO UC-420

Dr. F. Paoloni, Univ. of Wollongong, AUSTRALIA
Prof. M.H. Brennan, Univ. of Sydney, AUSTRALIA
Plasma Research Lab., Australian Nat. Univ., AUSTRALIA
Prof. I.R. Jones, Flinders Univ, AUSTRALIA
Prof. F. Cap, Inst. for Theoretical Physics, AUSTRIA
Prof. M. Heindler, Institut für Theoretische Physik, AUSTRIA
Prof. M. Goossens, Astronomisch Instituut, BELGIUM
Ecole Royale Militaire, Lab. de Phy. Plasmas, BELGIUM
Commission-European, DG. XII-Fusion Prog., BELGIUM
Prof. R. Boucique, Rijksuniversiteit Gent, BELGIUM
Dr. P.H. Sakanaka, Instituto Fisica, BRAZIL
Instituto De Pesquisas Espaciais-INPE, BRAZIL
Documents Office, Atomic Energy of Canada Ltd., CANADA
Dr. M.P. Bachynski, MPB Technologies, Inc., CANADA
Dr. H.M. Skarsgard, Univ. of Saskatchewan, CANADA
Prof. J. Teichmann, Univ. of Montreal, CANADA
Prof. S.R. Sreenivasan, Univ. of Calgary, CANADA
Prof. T.W. Johnston, INRS-Energie, CANADA
Dr. R. Bolton, Centre canadien de fusion magnétique, CANADA
Dr. C.R. James,, Univ. of Alberta, CANADA
Dr. P. Lukac, Komenskeho Universzita, CZECHOSLOVAKIA
The Librarian, Culham Laboratory, ENGLAND
Library, R61, Rutherford Appleton Laboratory, ENGLAND
Mrs. S.A. Hutchinson, JET Library, ENGLAND
P. Mähönen, Univ. of Helsinki, FINLAND
C. Mouttet, Lab. de Physique des Milieux Ionisés, FRANCE
J. Radet, CEN/CADARACHE - Bat 506, FRANCE
Ms. C. Rinni, Univ. of Ioannina, GREECE
Dr. T. Mual, Academy Bibliographic Ser., HONG KONG
Preprint Library, Hungarian Academy of Sci., HUNGARY
Dr. B. Das Gupta, Saha Inst. of Nuclear Physics, INDIA
Dr. P. Kaw, Inst. for Plasma Research, INDIA
Dr. P. Rosenau, Israel Inst. of Technology, ISRAEL
Librarian, International Center for Theo Physics, ITALY
Miss C. De Palo, Associazione EURATOM-ENEA , ITALY
Dr. G. Grosso, Istituto di Fisica del Plasma, ITALY
Dr. H. Yamato, Toshiba Res & Devel Center, JAPAN
Prof. I. Kawakami, Atomic Energy Res.Inst., JAPAN
Prof. K. Nishikawa, Hiroshima Univ., JAPAN
Director, Japan Atomic Energy Research Inst., JAPAN
Prof. S. Itoh, Kyushu Univ., JAPAN
Data and Planning Center, Nagoya Univ., JAPAN
Prof. S. Tanaka, Kyoto Univ., JAPAN
Library, Kyoto Univ., JAPAN
Prof. N. Inoue, Univ. of Tokyo, JAPAN
S. Mori, Technical Advisor, JAERI, JAPAN
O. Mitarai, Kumamoto Inst. of Technology, JAPAN
H. Jeong, Korea Advanced Energy Research Inst., KOREA
Prof. D.I. Choi, The Korea Adv. Inst. of Sci. & Tech., KOREA
Prof. B.S. Liley, Univ. of Waikato, NEW ZEALAND
Inst. of Plasma Physics, PEOPLE'S REPUBLIC OF CHINA
Librarian, Inst. of Physics, PEOPLE'S REPUBLIC OF CHINA
Library, Tsinghua Univ., PEOPLE'S REPUBLIC OF CHINA
Z. Li, S.W. Inst Physics, PEOPLE'S REPUBLIC OF CHINA
Prof. J.A.C. Cabral, Instituto Superior Tecnico, PORTUGAL
Dr. O. Petrus, AL I CUZA Univ., ROMANIA
Dr. J. de Villiers, Fusion Studies, AEC, S. AFRICA
Prof. M.A. Hellberg, Univ. of Natal, S. AFRICA
C.I.E.M.A.T, Fusion Division Library, SPAIN
Dr. L. Stenflo, Univ. of UMEA, SWEDEN
Library, Royal Inst. of Technology, SWEDEN
Prof. H. Wilhelmson, Chalmers Univ. of Tech., SWEDEN
Centre Phys. Des Plasmas, Ecole Polytech, SWITZERLAND
Bibliotheek, Inst. Voor Plasma-Fysica, THE NETHERLANDS
M. Durgut, Vice Chairman, Middle East Tech. Univ., TURKEY
Dr. D.D. Ryutov, Siberian Branch of Academy of Sci., USSR
Dr. G.A. Eliseev, Kurchatov Inst., USSR
Librarian, The Ukr.SSR Academy of Sciences, USSR
Dr. L.M. Kovrizhnykh, Inst. of General Physics, USSR
Kernforschungsanlage GmbH, Zentralbibliothek, W. GERMANY
Bibliothek, Inst. Für Plasmaforschung, W. GERMANY
Prof. K. Schindler, Ruhr-Universität Bochum, W. GERMANY
Dr. F. Wagner, (ASDEX), Max-Planck-Institut, W. GERMANY
Librarian, Max-Planck-Institut, W. GERMANY
Prof. R.K. Janev, Inst. of Physics, YUGOSLAVIA

END

DATE
FILMED
01/08/92