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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

PROGRESS REPORT

to the

International Nuclear Data Committee

from the

German Democratic Republic

Compiled by D. Seeliger

July 1983

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Readers are requested not to quote results contained herein without first consulting the appropriate authors.

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The present report contains abstracts of original investigations which are performed or in progress, as well as short reports on the activities of the nuclear data libraries in the GDR.

A more detailed information on all nuclear research activities is given in the annual report "Gemeinsamer Jahresbericht 1981" (ZfK - 488, October 1982), which recently was distributed to the INDC members.

During the period between the XII-th and XIII-th INDC-Meeting the coordinating group for nuclear data research "Arbeitsgemeinschaft Kerndaten" continued successful activities. Basing on the two big nuclear data libraries at the Technical University Dresden for neutron data and at the Central Institute of Isotope Techniques for nuclear structure and decay data the increasing number of requests from the nuclear data users could be covered. The continual support from the Nuclear Data Section of the IAEA is acknowledged.

C O N T E N T S

Doppler broadening of ^{238}U resonances in crystal lattices and molecular gas compared with the free-gas approximation

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and
Joint Institute for Nuclear Research Dubna+ (USSR)

For several chemical compounds of Uranium, transmission spectra have been measured with time-of-flight technique at the pulsed fast reactor IBR-30 with a procedure allowing the determination of differences between the spectra. The observed different Doppler broadening of low-lying resonances can not be interpreted in the frame of the commonly used free-gas-model. A description is possible with relatively simple weighted normal-mode frequency spectra of the crystal and molecular oscillations.

Direct comparisions of the Doppler broadening in crystals with the free-gas approximation are drawn for U-metal and UO_3 at 300 K and 600 K. The influence of intramolecular oscillations on the resonance shape is discussed for UF_6.

Furthermore the order of magnitude is indicated, as resonance parameters extracted by the shape analysis method, depend on these Doppler broadening procedures.

Calculation of fission neutron energy spectra and angular distributions in the framework of the cascade evaporation model

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The calculation of energy as well as angular distributions of fission neutrons on the base of the main emission mechanism, i.e. the evaporation from the fully accelerated fragments, represents an essential precondition for complex studies of fission neutron emission. A FORTRAN programme system was developed to deduce these data in the framework of the cascade evaporation model considering the excitation energy dependence of shell effects on the nuclear level density.

The calculation may be carried out for different scission configurations characterized by the fragment mass number ratio (asymmetry) and/or the total kinetic energy of the fragments (elongation). Results and conclusions concerning the spontaneous fission of ^{252}Cf were already described /1,2,3/.

Some additional effects which modify the calculated angular distributions and simulate scission neutron emission partially were studied:

i) the evaporation of neutrons during fragment acceleration /4/,
ii) the neutron emission from ^{5}He decay /5/.

In the case of induced fission reactions, the angular distributions may also be calculated with reference to the incidence particle direction.

/1/ H. Märten, D. Seeliger, B. Stobinski, Proc. Conf. on Nuclear Data for Science and Technology, Antwerp, 1982
/2/ H. Märten, D. Seeliger, submitted to J. of Phys. G
/3/ H. Märten, D. Neumann, D. Seeliger, Proc. XIIth Int. Conf. on the Interaction of Fast Neutrons with Nuclei, Gaußig, 1982
/4/ G.A. Pik-Pichak, Jad. Fiz. 10 (1969) 321
/5/ E. Cheifetz et al., Phys. Rev. Lett. 29 (1972) 805

Determination of Single-Level-Breit-Wigner parameters for resolved resonances in ^{28}Si+n

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Starting from parameters given in literature /1,2/ the resolved resonance structure in the total cross section for ^{28}Si+n /3/ has been fitted by a successive variation of Single-Level-Breit-Wigner parameters (SLBW) using the computer code SOKRES. Within the limitations of SLBW formalism a satisfactory approximation of the structure were achieved in the neutron incident energy range 10^{-5} eV to $1.5 \cdot 10^{6}$ eV by a final parameter set compiled in the table.

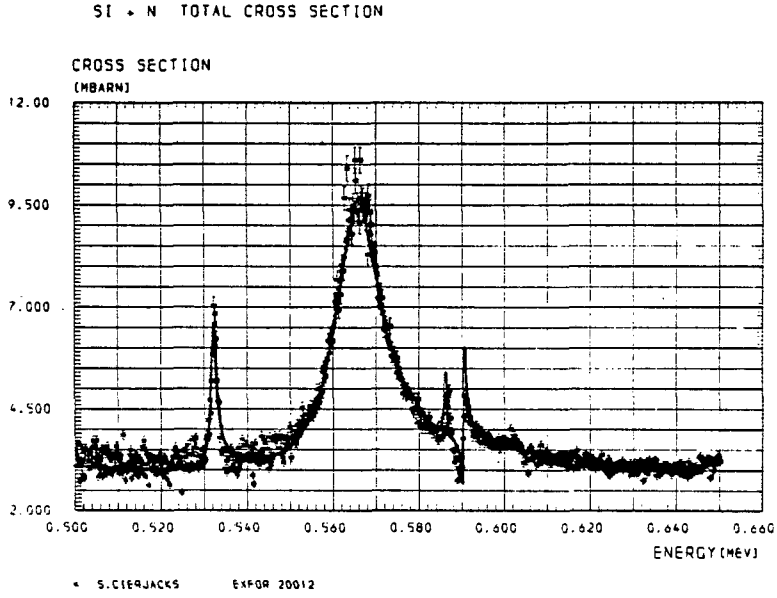

Fig. ^{28}Si+n total cross section in the energy range 0.5 to 0.65 MeV. The solid line has been calculated using SLBW resonance parameters compiled in the table.

Above 1.5 MeV the SLBW method fails the interpretation of the structure found experimentally /3/. An approved fit is possible by taking into account interference effects in terms of Multi-Level-formalisms /4/.

The dependence on temperature has been studied using the Ψ-χ-approximation yielding a negligable influence on the resonance structure only.

/1/ S.F. Mughabghab, D.I. Garber, report BNL-325, Vol. I, 1973
/2/ S. Igarasi, T. Nakagawa, Y. Kikuchi, T. Asami, T. Narita, report JAERI 1261, INDC(JAP)-45/L, 1979
/3/ S. Cierjacks, report KFK-1000, 1968, EXFOR acc. no. 20012
/4/ S. Cierjacks, private communication, 1982

Table: Compilation of SLBW resonance parameters describing the ^{28}Si+n total cross section up to 1.56 MeV neutron incident energy.

E_R/MeV	l	J	Γ/eV this work	E_R/MeV /1/	l /1/	J /1/	Γ/eV /1/
0.1865	0	1/2	29013.8	0.188	0	1/2	-
0.532	1	3/2	2000.8	0.5332	2	5/2	530±120
0.5635	1	3/2	14000	0.5662	1	3/2	10400±700
0.5655	1	3/2	11004	-	-	-	-
0.5865	1	1/2	103.3	0.587	1	1/2	800±300
0.5899	0	1/2	200	0.5927	1	1/2	400±200
0.602	1	1/2	34.1	0.6017	-	-	-
0.771	1	1/2	104	0.7722	-	-	-
0.8115	1	3/2	28000	0.8045	-	-	-
0.8145	1	3/2	32020.8	0.8162	1	3/2	27000±2000
0.8442	2	3/2	1507	0.8442	2	5/2	2500±800
0.8714	1	1/2	67	0.8714	-	-	<3800
0.9096	1	3/2	6502.3	0.9105	1	3/2	3000±500
0.959	1	3/2	95004.8	0.9667	1	1/2	90000±10000
1.016	1	3/2	200	1.016	-	-	1000
1.0415	1	3/2	1500	1.0417	1	1/2	1400±400
1.1615	0	1/2	2500	1.1639	0	1/2	1800
1.202	1	3/2	15000	1.2037	1	3/2	12000±3000
1.254	0	1/2	5000	1.252	0	1/2	7000±1000
1.263	1	3/2	2000	1.264	1	1/2	6000±4000
1.407	1	3/2	7000	1.4083	1	3/2	8000±2000
1.477	2	5/2	7000	1.4777	-	-	5500±500
1.51	1	1/2	600	1.5104	-	-	3500±700
1.5275	1	3/2	6000	1.5275	-	-	-

Investigation of direct reaction contributions to neutron-induced charged-particle emission from Silicon

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A systematical interpretation of experimental data for neutron-induced charged-particle emission in Si yields clearly evidence for the presence of direct reaction contributions to (n,p_i), (n,d_i) and (n,α_i) reactions /1/. These modes have been investigated in terms of charge and mass-exchange reaction models of knock-out and pick-up types resulting in following direct reaction contributions:

Neutron energy	p_0	p_1	d_0	d_1	d_2	d_3	d_4	d_5	d_6	α_0	α_1	α_2	α_3	α_4
~14 MeV	21	25	-	-	-	-	-	-	-	33	17	11	11	12
~21 MeV	-	-	65	60	43	35	25	27	34	78	-	-	-	-

A reasonable overall agreement and understanding from physics point of view can be achieved by an incoherent superposition of statistical and direct reaction components.

/1/ D. Hermsdorf, report INDC(GDR)-22/L, in press

Evaluation of neutron nuclear data for Silicon - MAT 2015 for the SOKRATOR library

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A complete file of evaluated neutron nuclear data for Silicon has been created containing about 7800 records. Special attention was given to neutron and charged-particle production cross sections /1/.

The numerical figures were formatted in ENDF/B-V format. A description of the evaluation procedure and the contents of MAT 2015 has been prepared for publication /2/.

At present the data will be checked against misprints and numerical consistency using the codes CHECKER-5 and FIZCON-5. Tests against physics inconsistencies basing on calculations of integral data are underway. The final corrected version of MAT 2015 will be available at the end of this year.

/1/ D. Hermsdorf, report INDC(GDR)-22/L, in press
/2/ D. Hermsdorf (ed.), report INDC(GDR)-20/L, in press

SOKRES - A computer code for the calculation of resolved resonances in terms of Single-Level-Breit-Wigner formalism

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Dealing with clearly resolved resonances ($\Gamma \gg D$) the Single-Level-Breit-Wigner formalism (SLBW) gives a satisfactory approximation of the structure in cross sections found experimentally.

In the case of neutron elastic scattering and neutron-induced reactions (capture and fission) the relevant formulae have been defined in the format description for ENDF/B /1/. According to these a computer code has been written to calculate point-wise cross sections proceeding from SLBW resonance parameters for elastic scattering, capture and fission including as well as interferences between potential and resonance scattering and a "background" to take into account 1/v-laws for capture and fission cross sections.

The influence of the temperature on the resonance shapes can be simulated in terms of the ψ-χ-approximation.

The code is written in FORTRAN for a BESM-6 computer and should be used in two operation modes:

i) determination of SLBW resonance parameters by fitting experimental cross sections

or

ii) calculation of point-wise cross sections by use of a given SLBW parameter set formatted in ENDF/B-V format.

/1/ D. Garber, C. Dunford, S. Pearlstein, report BNL-NCS-50496 (ENDF 102), 1975

A simple model for calculation of fast neutron-induced γ-ray spectra

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A paper has been submitted to Nucl. Sci. Eng. with following abstract:

A semiempirical model, the so-called R-parameter model, introduced by Howerton and Plechaty has been proved to be a simple but, nevertheless, a very succesful formalism for the description of γ-ray spectra emitted in the course of nuclear reactions induced by fast neutrons. By the single parameter R the γ-ray spectrum will be predicted with a satisfying reliability in a wide range of nuclear masses and neutron incidence energies. The formalism is limited at neutron incidence energies below the (n,2n)-threshold. Above this energy a modified ansatz proposed by the present work yields good results.

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Determination of effective absorption cross-sections of structure materials

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The measurements were performed in a special fast substituted lattice (SEG-IV) with energy-independent adjoint neutron flux /1/. This enabled us to use the pile-oscillator method, because in that case the moderation term of the reactivity-worth becomes zero and the absorption term is directly proportional to the effective absorption cross-section of the material under investigation. These cross-sections were determined relative to ^{10}B as a standard and compared with calculated ones (table 1).

Table 1: C/E-values for effective absorption cross-sections

	σ_{exp}[mb]	ABBN-64	ABBN-78	JFS-II	BARC	KEDAK-3	UKNDL
Ti	42±6	0.95	-	-	-	-	-
Cr	17.7±2	1.18	1.24	1.33	1.6	0.83	1.18
Mn	255±40	-	0.82	0.95	-	-	-
Fe	14.1±2	0.81	1.15	1.15	2.2	1.9	-
Ni	36.4±4	0.87	1.12	0.98	2.6	0.98	-
Cu	82±8	1.22	-	1.11	-	-	-
Zr	33±5	1.01	-	-	-	-	1.07
Nb	282±34	1.56	-	-	-	-	-

In general chromium is calculated too high by about 25 %, whereas the data for manganese (especially those for resonance shielding) are underestimated. For iron the spread of the data is rather high, the best agreement (C/E = 1.07) being achieved with evaluated data of the Technical University Dresden /2/. Obviously, the Indian set BARC (Garg, 1976), which is based on the ENDF-B/III, is the worst concerning the nuclides Cr, Fe and Ni.

/1/ K. Fährmann, E. Lehmann, Kernenergie 24 (1981) 431
/2/ V.M. Bychkov, V.V. Vozyakov, V.N. Manokhin, F. Smoll, P. Rösner, D. Seeliger, D. Hermsdorf, Yad. Konst. 1 (36), 1980, p. 65

Use of the database for nuclear structure and decay data

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The content of the database for nuclear structure and decay data at the Central Institute for Isotope and Radiation Research (ZfI) Leipzig has already been described /1/. In the period January to December 1981 no changes had been made on principle, but all files (mentioned in /1/) had been replaced by their most modern version.

The major activity in 1981 was the implementation of the computer code MEDLIST (originated at ORNL) received by support of the IAEA at the institutes own ES 1040 computer.

According to /2/ MEDLIST prepares tables of atomic and nuclear radiations based on ENSDF data sets. The code calculates K, L, X-ray intensities and also conversion-electron radiations. Detailed information about MEDLIST was given by Martin and Kocher /3,4/.

During the implementation of MEDLIST at the institutes ES 1040 computer some changes had to be made. One difficulty e.g. occured in replacing the missed subroutine CORE. For our users only changes in the character-set (replacement of Greek Letters, super- and subscript) are visible. An example of a MEDLIST prepared ENSDF data set is given in fig. 1.

In 1982 this code will be used in answering routine requests for decay data. Some experiments in changing internal parameters of MEDLIST will be undertaken in 1982. Still in 1981 already 19 datasets of ENSDF decay data had been prepared for users of our institute using MEDLIST.

The overall request statistics for the period January to December 1981 is the following:

- user requests 26
- datasets and references printed 877
- surches in datafiles 41
- special catalogues printed upon user request 2.

233NP EC DECAY (36.2 M) I(MIN)= 0.10%

RADIATION TYPE	ENERGY (KEV)	INTENSITY (%)	D(G*RAD/UCI*H)
AUGER*L	9.89	34 5	0.0072
AUGER*K	72.6	1.7 13	0.0026
X*RAY L	13.6	44 5	0.0126
X*RAY KA2	94.6050 20	21.9 5	0.0442
X*RAY KA1	98.4390 20	35.6 7	0.0746
X*RAY KB	111	16.6 4	0.0392
G 9	234.3 5	0.154 7	0.0008
G 16	280.5 5	0.133 7	0.0008
G 17	299.1 5	0.50 7	0.0032
G 19	312.1 3	0.7	0.0047
G 25	506.5 5	0.154 21	0.0017
G 26	540.9 4	0.286 14	0.0033

24 WEAK G'S OMITTED (SUM(IG)= 0.78284%)

Fig. 1 MEDLIST prepared ENSDF data set 233NP electron capture decay

In addition to this activites also in 1981 abstracts of GDR reports and articles were prepared and sent to the LIJAF Institute Leningrad for including them in the international reference file and if possible in NSR. In 1981 62 references had been prepared.

/1/ Jankowski, Friedrich, Letz, Installation of a database for Nuclear Structure and Decay Data, INDC(GDR)-16/G

/2/ Ewbank, Schmorak, ENSDF - A Manual for the Preparation of Datasets, ORNL-5054/R1

/3/ M.J. Martin, Nuclear Data for Selected Radionuclides, ORNL-5114

/4/ D.C. Kocher, Nuclear Decay Data for Radionuclides occuring in Routine Releases from Nuclear Fuel Cycle Facilities, ORNL/NUREG/TM-102

Variation of the nuclear deexcitation rate of Tc-99m in different chemical states

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A systematic experimental and theoretical study of the nuclear deexcitation rate of Tc-99m in the halogen and oxy complex ions TcX_6^{2-} and TcO_4^-, respectively, (X=I, Br, Cl, F) as well as in the metal was carried through. Preparation of the halogen complexes occured by standard methods /1/; the measurements were accomplished by a semidifferential approach /2/. The measuring results for X=Cl, Br, I, and TcO_4^- were published /3/. The X_α-SW-SCF-treatment /4/ of the systems studied showed an excellent agreement between theoretical and experimental values for X=Br, I and TcO_4^- and a discrepancy for X=Cl. The reason for the latter was found to be a chemical instability of our $^{99m}TcCl_6^{2-}$ compound. An improved preparation procedure /5/ gave a chemical stable $TcCl_6^{2-}$ complex, for which we measured the theoretically expected decay constant variation.

Our experiments on the metallic Tc-99m, details of which are to be published /6/, confirmed the measuring value of Bainbridge /7/, whereas the result of the X_α treatment /8/ speaks in favour of Mazaki's measurement.

Our experiments on TcF_6^{2-}, to be published /6/, confirm the tendency of the decay constant of Tc-99m in the halogen complexes predicted by the X_α theory /4/, but a quantitative agreement could not be found, in contrast to the I, Br, Cl cases.

Experiments /9/ and X_α calculations on the decay constant variation of the radiopharmaceutical Tc-99m Bis(meso-dimercapto-succinato)oxotechnetate(V) were published /10/.

/1/ K. Schwochau, Angew. Chem. 76 (1964) 9-19
/2/ P. Huber et al., Phys. Lett. 27B (1968) 86-87

/3/ M. Nagel et al., Z. Naturforsch. 33a (1978) 1050-1055
/4/ E. Hartmann et al., Z. Phys. A290 (1979) 349-353
/5/ K.-P. Dostal, B. Bayerl, Z. Naturforsch. 35a (1980) 894-895
/6/ G. Brunner et al., Z. Phys. A, to be published
/7/ K.T. Bainbridge et al., Phys. Rev. 90 (1953) 430-439
/8/ E. Hartmann, G. Seifert, Phys. stat. sol. (b) 100 (1980) 589-594
/9/ B. Johannsen et al., Radiochem. Radioanal. Letters 47 (1981) 57-62
/10/ E. Hartmann, G. Mocker, ZfK-Bericht 1981

Precision measurement of the decay constant of ^{99m}Tc in the pertechnetate ion by means of a variational method*

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In radioactive decay a linear relation exists between the measured counting rate (uncorrected for dead-time and background) and the background-corrected counting rate multiplicated by the factor $e^{\lambda t}$. Varying the decay constant λ, this connection gets nonlinear, and the statistical error of the slope, estimated by means of linear regression, increases. Therefore, the statistical error of the slope has a minimum at the wanted true value of decay constant. In this way the decay constant of ^{99m}Tc in the pertechnetate ion was found to be $\lambda=(3,20525\pm0.00093)\cdot10^{-5}s^{-1}$ respectively $T_{1/2}=(6,0070\pm0,0018)h$.

*This work has been published in Isotopenpraxis, 18 (1982) 201

Measurement of the halflife of ^{125}I

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The halflife of five ^{125}I sources was determined by a two-NaI(Tl)-scintillation-detector-method to minimize geometrical and other errors. The total measuring time was 130d (about two halflifes of ^{125}I).

After testing the clean exponential behaviour of the background- and dead-time-corrected counting rates as a function of the time we got a value of

$$T_{1/2} = (59.54 \pm 0.02)d$$

for the ^{125}I halflife. The error is the standard deviation of the mean value of the five sources. It agrees with the standard deviation of the slope of the single decay curves in logarithmic representation, determined by linear regression.

The result may be compared with the value given in /1/ $T_{1/2}=(59.666 \pm 0.016)d$, to our knowledge the exactest result among the hitherto published ^{125}I halflifes.

/1/ W. Kündig, P.E. Müller, Helv. Phys. Acta 52 (1979) 555

Effect of the chemical structure on the electron density at the iodine nucleus

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The X_α-SW method /1/ was employed to deduce estimates of the differences in the electron-charge densities at the iodine nucleus in the ions ICl_4^-, IO_3^-, I^-, IO_4^- and IO_6^{5-}. On the basis of these estimates some assertions were deduced to the calibration problem of the Mössbauer nuclide ^{129}I and to the halflife variations in the EC (^{123}I and ^{125}I) and IC (^{129}I) decay.

The deduced alteration of the mean-square nuclear charge radius of the Mössbauer nuclide ^{129}I of $(20.0\pm3.)10^{-3}fm^2$ is in a rather good agreement with values derived by other methods. Our estimates are also consistent with experimental data for the chemical effect on the IC of ^{129}I /2/ and EC of ^{123}I /3/. The measuring values for the chemical EC variation in ^{125}I compounds /4/, however, differ from the corresponding theoretical estimates by a factor greater than 3. The inclusion of overlap and exchange correction /5/ improves the agreement between theory and experiment for the EC data of ^{123}I but the aforementioned discrepancy for the EC of ^{125}I becomes even more pronounced.

In order to test the systematics of nuclear-near electron densities we remeasured the chemically induced EC decay variation of ^{125}I. The measurements were accomplished by a semidifferential approach /6/. The measuring values show a good agreement with the theoretical results. The results are published in /7,8/.

/1/ J.C. Slater, Quantum theory of molecules and solids, vol. 4 (Mc Graw Hill, New York, 1974)
/2/ W.J.J. Spijkervet, F. Pleiter, Hyp. Int. 7 (1979) 285
/3/ J. Ladrière, M. Cogneau, A. Meykens, J. Phys. 41 (1980) C1-131

/4/ W. Kündig, P.E. Müller, Helv. Phys. Acta 52 (1979) 555

/5/ K.V. Makariunas, Izv. Akad. Nauk SSSR Ser. Fiz. 43 (1979) 96

/6/ P. Huber et al., Phys. Lett. 27B (1968) 86

/7/ E. Hartmann, Ch. Eifrig, Chem. Phys. 58 (1981) 283

/8/ E. Hartmann, Ch. Eifrig, G. Brunner, accepted for publication in Hyp. Int.

Computer code for calculation of ICC for all atomic shells including higher order corrections

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A computer code /1/ for calculation of ICC for all atomic shells, originally written for purposes of estimation of chemical shifts of the ICC, was extended to include corrections of higher order of pertubation theory according to the theory of Krutov /2/.

For the highly converted E3 transitions in Tc-99m and U-235m the total ICC in second (usual) and in fourth order calculated by /1/ amount to /3/

	$\alpha^{(2)}$	$\alpha^{(4)}$
Tc-99m	$1.38 \cdot 10^{10}$	$1.37 \cdot 10^{10}$
U-235m	$4.82 \cdot 10^{20}$	$3.19 \cdot 10^{15}$

The decrease of the ICC in fourth order is caused primarily by a corresponding increase of the transition probability towards radiative deexcitation ("electron bridge" /2/) due to the mere presence of the electron cloud.

The nonresonance contributions to the transition probability, enclosed in our calculations /4/, turn out to be negligible in these cases.

An advanced version /5/ of /1/, still unpublished, yields second order ICC values, which excellently agree with those of Roesel et al. /5,6/.

/1/ R. Der et al., Comp. Phys. Comm. 18 (1979) 401-410
/2/ V.A. Krutov, V.N. Fomenko, Ann. Phys. (Leipzig) 21 (1968) 291-302
/3/ D. Hinneburg et al., Z. Phys. A291 (1979) 113-115
/4/ D. Hinneburg, Z. Phys. A300 (1981) 129-132
/5/ D. Hinneburg, Thesis, Leipzig (1982)
/6/ F. Roesel et al., Atomic Data and Nucl. Data Tables 21 (1978) 91

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