

NKE: an electronic nuclide chart

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<http://snow.prohosting.com/roeug/index.htm> or <http://www.websamba.com/roeug/default.htm> (May, 2003)

NKE program serves as a tool to visualize base nuclear physical properties (half-life, neutron reaction cross-sections, the data on radioactive decay channels, etc.) and to analyze the information on the total radioactive isotope set as a single whole. Such analysis may appear extremely useful at a choice of new perspective nuclides for the specific practical application. The convenient form of such information representation is the format of widely known nuclide chart ('Karlsruher Nuklidkarte'). It was used during development of the program user interface. Being a component of ORIP_XXI software suite, whose tasks include the solving of the problems concerning nuclide transmutation calculations in neutron irradiations, NKE can be used as a stand-alone utility. While the computational program of the software suite (ChainSolver code) is used for the solving of the nonlinear differential equations systems describing dynamics of nuclide accumulations in the presence of radioactive decay of isotopes, neutron flux, and both self-shielding and depressions, NKE displays the detailed information about nuclides contained in ORIP_XXI software suite data file (the file is common for all software suite programs). Also NKE displays the information on such properties of radioactive elements (in general not necessary for transmutation calculations) as characteristics of radioactive radiation. On the basis of the displayed data, the chain searching code (ChainFinder) builds nuclide transmutation chains (based on the starting isotope and the target one, taking into account, if necessary, neutron reactions and neutron induced fission of heavy nuclei).

The data file contains nuclear properties and the decay radiation data for more than 2800 nuclides with nuclear weights from 1 up to 293 (a charge of a nucleus from 1 up to 118) and the characteristics of chemical elements. In the software suite the data are stored in a format of free object-oriented database that enables to achieve enough high program efficiency even on rather slow computers at very small data file size (near 2 Mb).

The main program window Fig.1 is a nuclides chart. The chart is the program skeleton. Special actions with the chart (mouse single and double clicks, menu items selection) serve to call various user-end subroutines. The friendly user interface allows choosing the information displayed on a nuclide chart. There is an opportunity of fast moving to a desired nuclide.

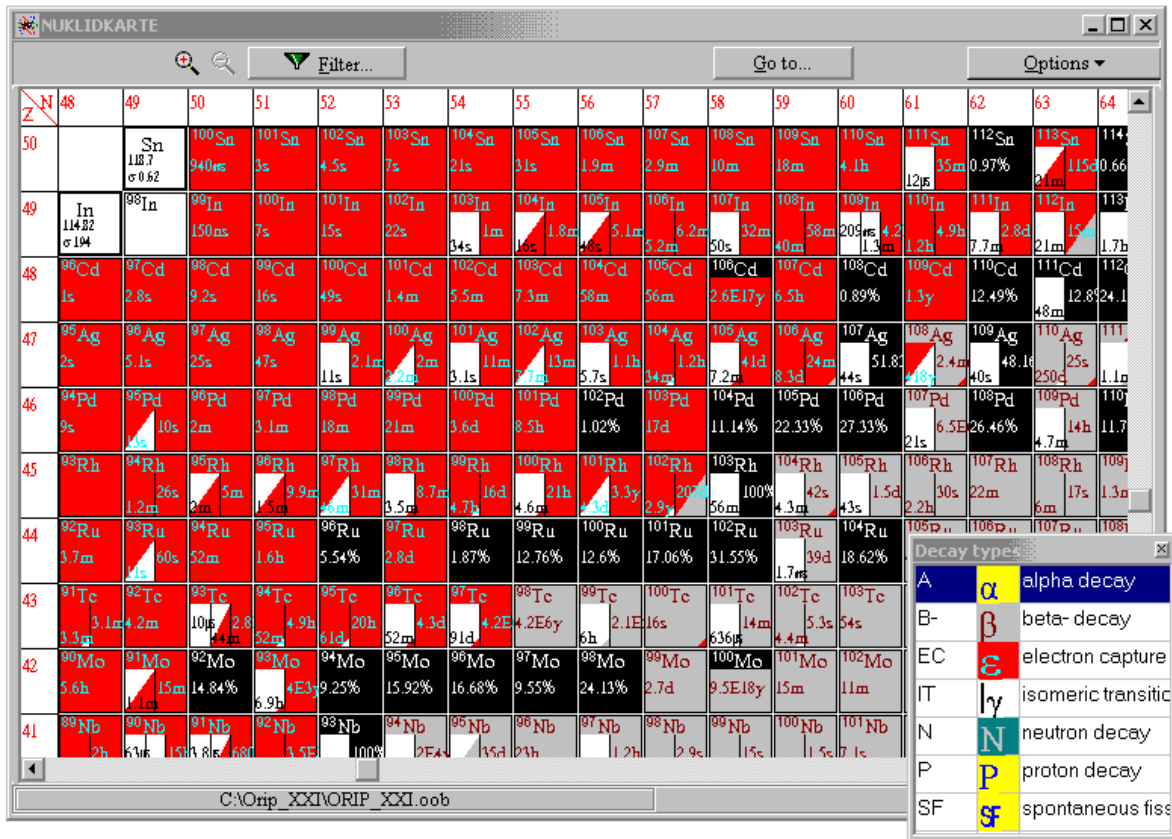


Fig 1. The main window of NKE program (with the legend)

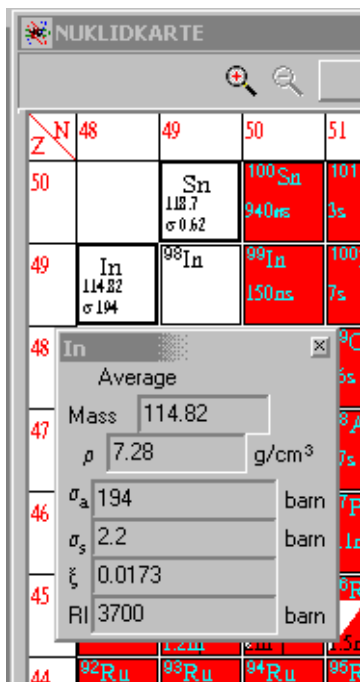


Fig.2. The element data in NKE program

Outputs for elements (mouse double click in an element box) are following: average relative nuclear weight (on the oxygen scale), mass density, scattering and absorption cross-sections for thermal neutrons, average energy loss of a neutron at a collision with the nucleus in terms of lethargy x , resonance integral for neutron absorption RI (Fig.2). The data are taken from book [1] and checked on an available file, which refers to Handbook of Chemistry [2].

$$x = \left\langle \ln\left(\frac{E_0}{E}\right) \right\rangle, \quad \text{where } E_0 \text{ and } E - \text{energy of a neutron before and after collision, respectively}$$

$$RI = \int \frac{\sigma_a(E)}{E} dE, \quad \text{where } \sigma_a \text{ is a neutron absorption cross-section.}$$

Such data give an opportunity to carry out two group neutron transport evaluations.

The program displays the detailed information on nuclides (including isomer states) Fig.3,5-7. On mouse double click in a nuclide cell of the chart the common information about the nuclide (including the abundance in a nature mixture of isotopes) is shown. For any isomeric state the user has an opportunity to request the data on cross-sections (including threshold reactions ones), the data on yields at heavy nucleus fission, alpha, electron, gamma lines and beta and positron spectra parameters (including the estimation of ionizing gamma-constant K_γ , $R \cdot \text{cm}^2 \cdot \text{hour}^{-1} \cdot \text{mCi}^{-1}$)).

For radioactive states there is an opportunity to calculate the time disintegration User gives time interval (in convenient units) for which it is necessary to calculate residual concentration of a decaying isotope (Fig.4).

The data were taken from the following public sources of the information: the abundance of isotopes, states half-life, thermal cross-sections and resonance integrals (RI, for infinite dilution [3]) cross-sections for a neutron capture and fission are from program PCNUDAT [4]. PCNUDAT is the MS Windows version of the program for a data access of the National Nuclear Data Centre (NNDC Online Data Service data base NUDAT). It contains the data on the ground and metastable nuclide states, the half-life of nuclides, the data on radioactive isotope decays, levels of energy and nuclear state spins.

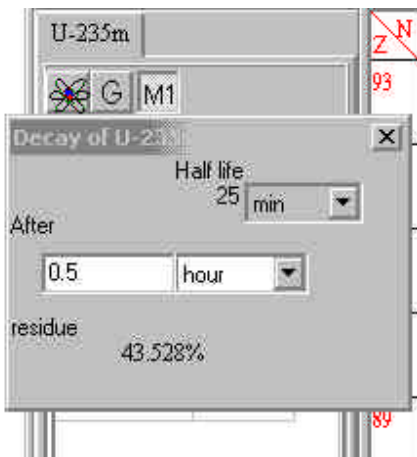


Fig.4. The decaycalculator

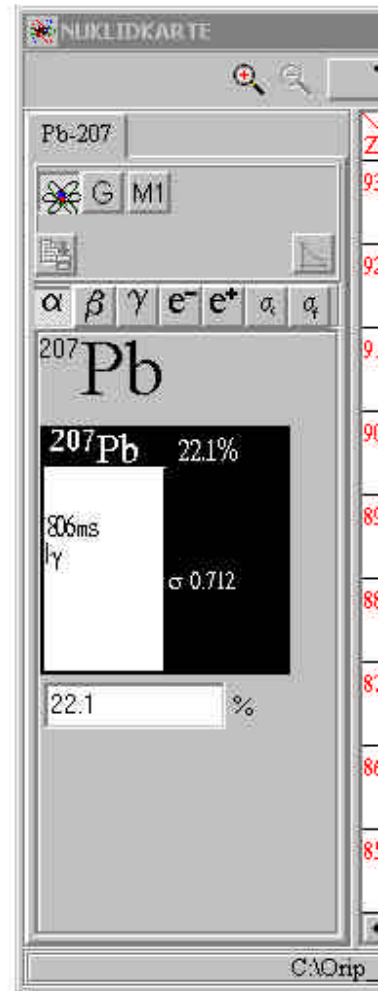


Fig.3 Detailed information for a nuclide (the common view)

NUDAT data were selected from publications [5-13] by NNDC. Cross-sections of threshold reactions were received by convolution of a fission spectrum with the pointwise cross-section and are published in the Internet on pages of KAERI (Korea), BNL (USA), ISIS (UK), Ruhr University Bochum (Germany) [14]. The above sources include estimated data received by the analysis of values

published in various pointwise libraries of neutron cross-sections. These pointwise cross-sections are also the base of NGATLAS library [15], which contains values of neutron reaction cross-sections for isotopes up to Cm inclusive.

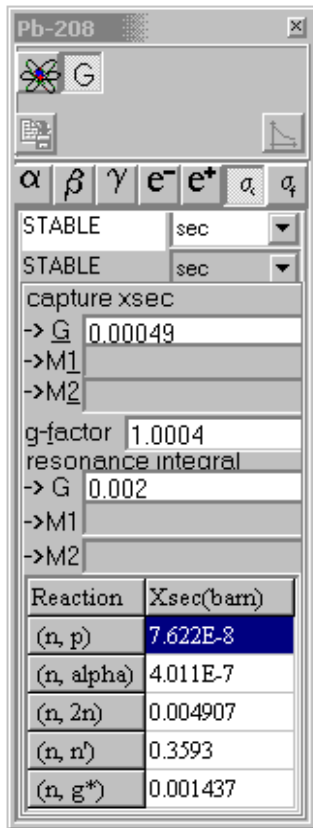


Fig.5. Neutron reaction cross-sections

The program data include cross-sections for almost 740 isotopes with half-life more than 12 hours; neutron reaction cross-sections for the ground, the first, and the second metastable states are shown separately (if the data are present). Thus, there are values for almost thousand channels of reactions in NGATLAS. Power dependences of "isomer channels of reactions partitioning" (the cases when at neutron reaction various long-living isomer states of the isotope are possible) are based on combination of the experimental information and empirical techniques. Pointwise cross-sections with experimental data also can be found with their comparison at [16].

Products yields of heavy nucleus fissions (both for a thermal spectrum of neutrons and for a fast spectrum) were taken from the publication [17], which contains recommended distributions of nuclear weights and charges of

nucleus of fission products, received from the analysis of experimental data on the fission, published in the open literature. The publication serves also as the initial document for the subsequent estimations of yields that are resulted in files ENDF/B-VI (ENDF-Evaluated Nuclear Data Files, which are accessible in National Nuclear Data Center [18]). Various data on fission product yields (the experimental, calculated and recommended values, and both individual and cumulative yields for each) are given in [17]. The individual yield is the probability of the product formation per one hundred fissions.

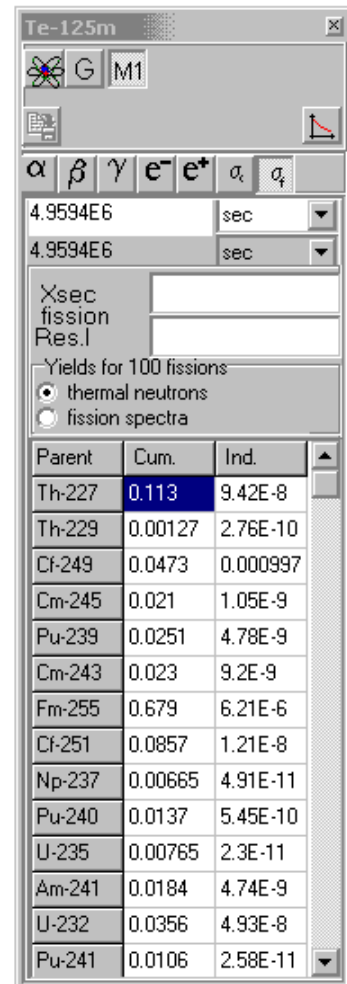


Fig.6. Fission yields of the nuclide state

The cumulative yield is the sum of the isotope individual yields and individual yields of all its predecessors in a radioactive decay chain. Calculated values are received by calculation of yields on various models of nucleus fission and decays. Because of the output of all six values for one isotope is not reasonable; the recommended cumulative and individual yields received by authors [17] from experimental and calculated in view of preservation laws data are displayed in NKE program.

To mine the information about alpha, gamma and electron lines, and both beta- and positron spectra the data of Radiation Decay program [19] were used. In Radiation Decay code documentation it is underlined that the data for the code are from Radiation Safety Information Computational Center (RSICC, earlier RSIC- Radiation Shielding Information Center [20]) and meet publications [21]. $K\gamma$ values in NKE program (ionizing gamma-constant, $R\cdot cm^2\cdot hour^{-1}\cdot mCi^{-1}$) are calculated with the technique from V.P.Mashkov and A.V.Kudrjajtsev book [22].

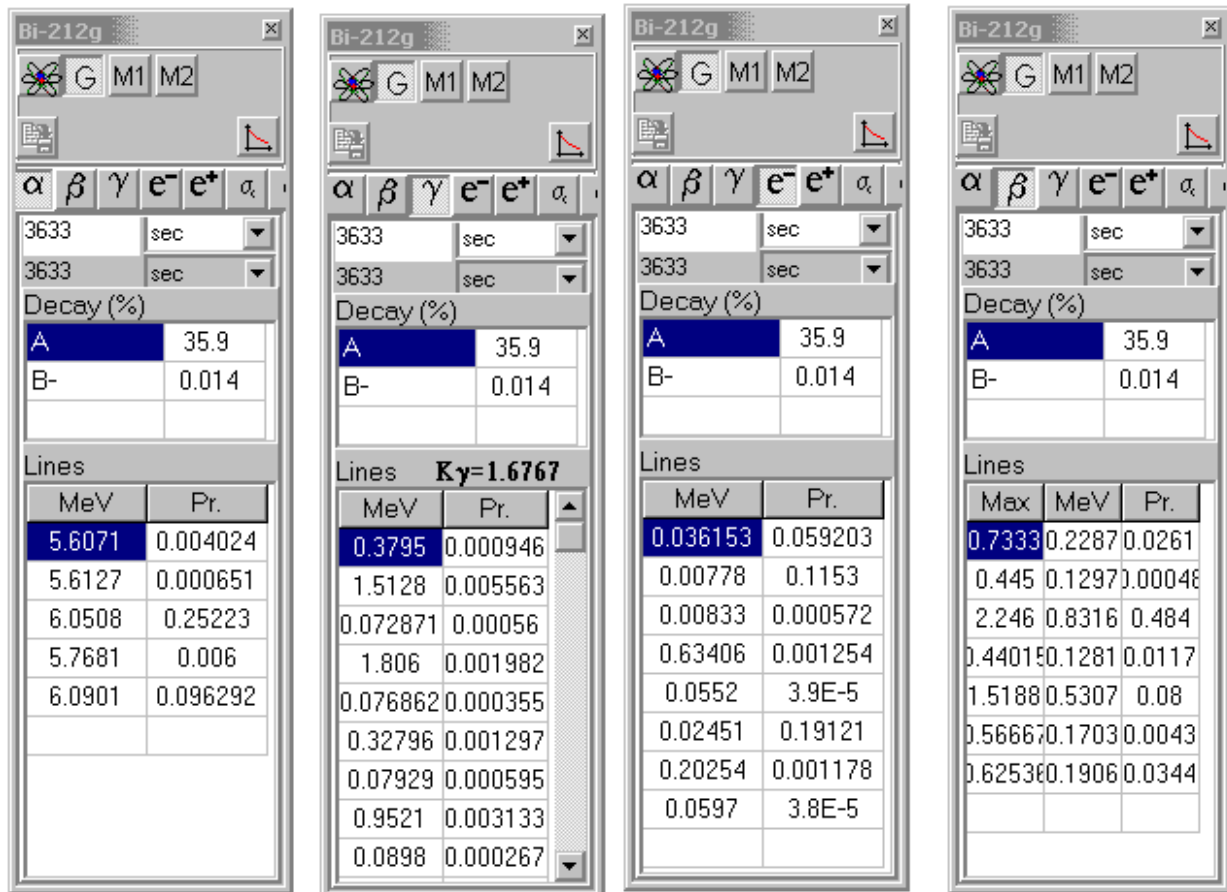


Fig.7. The information about alpha, gamma, electron lines and beta- spectra

The program can perform complex searches for the analysis of the whole data available in ORIP_XXI software suite data file. The dialogue (Fig.8) allows the search filter conditions

formulating, which are describing what isomer states should be submitted in sampling. The user sets selection conditions (may be, for several isotopes characteristics). At definition of several filter conditions it is possible to use 'AND' or else 'OR' logic operators. See Fig.8 for a filter example of the selection and the corresponding state list output. It was required to find isotopes that are beta- particles sources but the radioactive decay of these states is not accompanied by gamma radiation. Such nuclides may appear extremely perspective for medical application.

State	Half life
Be-10	1.5E6y
C-14	5.7E3y
Si-32	172y
P-32	14.3d
P-33	25.3d
S-35	87.4d
Ar-39	269y
Ar-42	32.9y
Mn-60g	51s
Ni-63	100y
Ni-66	2.28d
Se-79g	1.1E6y
Rb-87	4.7E10y
Sr-90	28.8y
Ru-106	1.02y
In-115g	4.4E14y
Sn-121g	1.13d
Cs-135g	2.3E6y
Re-187	4.3E10y

Fig.8. Selection of nuclide states interesting for the user

Program NKE should be mainly considered as a part of ORIP_XXI software suite displaying the initial data for calculation of nuclide chains. That is why the program was developed to be maximum open and easily scaled that was achieved by means of Borland Object Pascal object-oriented coding language. The developed architecture of program classes enables to use their object interface parts in practically any algorithms. The nuclide chart cells are painted in a separate program thread to increase the data visualization speed and quality.

Program NKE may be used as the stand-alone utility (together with ORIP_XXI software suite data file).

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