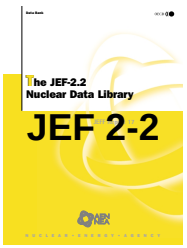

JEF/DOC-813

REVIEW OF DECAY DATA CHECKING METHODS

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Summary

Evaluated decay data files in ENDF-6 format are assembled in major libraries such as JEF2.2. This review examines methods for checking the internal consistency of such data, and it assesses the present features of two checking codes, OKDK and FIZCON. It recommends that FIZCON should be adopted as the code for checking decay data files for the JEF project, with the necessary code developments being made to meet the outstanding requirements.

1. INTRODUCTION

Evaluated decay data files are now assembled in major libraries like JEF2.2 [1]. The evaluation is performed in different laboratories/countries collaborating in the production of the library. In the UK the COGEND computer code [2] is applied to evaluated decay data and generates decay files in ENDF-6 [3] format. During this process COGEND adds spectral data for X-rays and electrons using physics methods programmed within the code. It also calculates mean spectral and decay energies. Finally it performs a check on the overall energy balance within the evaluation:-

(Effective Q-value)-(Calculated Q-value)<1% of the Effective Q-value.

where

$$\text{Effective Q-value} = \sum_{r}^{All\ Decay\ Modes} Q_r B_r$$

i.e. the sum of the decay energy times the Branching Fraction of each decay mode,

and

$$\text{Calculated Q-value} = \sum_{i=1}^{all\ \gamma} E_{\gamma i} P_{\gamma i} + \sum_{j=1}^{all\ \beta^-} E_{\beta^- j} P_{\beta^- j} + \sum_{k=1}^{all\ \beta^+} E_{\beta^+ k} P_{\beta^+ k} \ldots$$

where the *E* terms are transition energies associated with each emitted quantity and the *P* terms are the overall intensity of the emitted particles/quanta.

Hence UK evaluations are likely to have been assessed for consistency, but many problems can occur during assembly. Evaluations from other sources will not have been assembled in the same way. Hence all evaluators are now recommended to apply the overall energy balance check [4]. As part of this exercise, work on a prototype code, OKDK [5], was started at Winfrith, with support from British Nuclear Fuels.

Modern QA procedures [6] are now applied to the assembly of neutron cross section evaluations and are likely to be extended to decay files. The procedures recommend application of the BNL code FIZCON [7]. This code includes features to check decay files but the documentation is somewhat limited.

Further study of internal consistency of decay evaluations is now taking place at Winfrith with BNFL and OECD support. The initial stage of the work, described in this paper, is to assess present features in OKDK and FIZCON and to recommend further development that should take place.

2. DECAY DATA FILES

In the ENDF-6 format, radioactive decay data are given in File MF=8 under MT=457. The format guide [3] gives a detailed description of the data, but a brief outline is given here in order to define the quantities involved in the checking process.

The first part of the data is a collection of general information about the nuclide. This includes three average decay energies: $E_{"\beta"}$, $E_{"\gamma"}$ and $E_{"\alpha"}$. These are for use in calculating decay heat, and they represent the average amount of energy of each type emitted per decay.

The "β" term encompasses all electron radiation, including β^-, β^+, internal conversion electrons and Auger electrons. The "γ" term encompasses all electromagnetic radiation including gamma-rays, X-rays and annihilation radiation. The "α" term encompasses all heavy particles including alpha particles, protons, neutrons, spontaneous fission fragments and recoiling nuclei. Because these quantities are intended for heating calculations, neutrino energies are not included.

The second part of the data provides information about each mode of decay. The possible modes are shown in Table 1. The data given for each mode include the branching fraction and a Q value.

The third part of the data gives information about each type of radiation emitted. The possible radiation types are listed in Table 2. For each radiation type, the energy spectrum is given in the form of discrete lines or a continuum or both. Normalisation factors are given to define the absolute intensity (per decay). The decay mode giving rise to the emitted radiation is specified for each discrete energy or continuum distribution. For each type of radiation, an average decay energy, ER_{AV}, is given. This is the average amount of energy of this type emitted per decay. These values are provided for decay heat applications, and therefore exclude neutrino energy; they are the components of the $E_{"\beta"}$, $E_{"\gamma"}$ and $E_{"\alpha"}$ quantities given in the first part of the data.

Table 1 Decay Modes

RTYP		Mode of Decay
1	β^-	Beta decay
2	e.c./β^+	Electron Capture and/or positron emission
3	IT	Isomeric Transition
4	α	Alpha decay
5	n	Neutron emission (not “delayed neutron decay”)
6	SF	Spontaneous fission
7	p	Proton emission
10	-	Unknown origin
Multiple particle decay (examples):		
1.5	β^-,n	Beta decay followed by neutron emission ("delayed neutron decay")
1.4	β^-,α	Beta decay followed by alpha emission (e.g. ^{16}N decay)
2.4	β^+,α	Positron decay followed by alpha emission

Table 2 Radiation Types

STYP		Radiation Type
0	γ	Gamma Rays
1	β^-	Beta Rays
2	e.c./β^+	Electron Capture and/or positron emission
3	-	-
4	α	Alpha Particles
5	n	Neutrons
6	SF	Spontaneous fission fragments
7	p	Protons
8	e^-	Discrete electrons
9	x	X-rays and annihilation radiation (photons not arising as transitions between nuclear states)

3. OUTLINE OF REQUIRED CHECKS

Checks are required to ensure that energy distributions are consistent with the total energy values that are given in the file. This section outlines three such checks in a general form. Subsequent sections will discuss how they need to be modified in certain cases. Table 3 lists the main quantities involved, indicating the symbols used in the ENDF-6 format guide and also the notation used locally in this document.

Table 3 Definition of Symbols

ENDF-6 symbol	Local symbol	Description
$E_{"x"}$	$\overline{E}_{"x"}$	Average amount of energy of type "x" emitted per decay, where "x" = "β" (all electron radiation),"γ" (all electromagnetic radiation) and "α" (all heavy particles).
RTYP	r	Decay mode (see Table 1)
Q	Q_r	Q value for mode r decay
BR	B_r	Branching fraction, i.e. the fraction of decays that proceed by mode r
STYP	s	Radiation type (see Table 2)
FD	-	Discrete spectrum normalisation factor
RI	-	Relative intensity for a discrete spectrum line
ER	E_{si}	The ith discrete energy for radiation type s
FD*RI	P_{si}	Absolute intensity (per decay) of the radiation at energy E_{si}
FC	-	Continuum spectrum normalisation factor (= absolute intensity)
RP(E)	-	Spectrum for the continuum component (normalised so that $\int RP(E)dE = 1$)
FC*RP(E)	$P_{sc}(E)$	Spectrum for the continuum component of radiation type s (normalised so that $\int P_{sc}(E)dE = \text{absolute intensity}$)
ER_{AV}	$\overline{E}_s$	Average amount of energy of radiation type s emitted per decay
-	$\overline{E}_{si}$	Average amount of energy emitted per decay, associated with the ith discrete energy of radiation type s
-	$\tilde{E}_{si}$	Amount of energy associated with the ith discrete energy of radiation type s (for Q value check)

3.1 Check 1: Average decay energy for each radiation type

For each radiation type (i.e. STYP), the average amount of emitted energy, ER_{AV}, should be consistent with the spectrum data for that radiation type. This means that it should be possible to reproduce the ER_{AV} value by a summation over the discrete energy lines and an integration over the continuum spectrum. This condition may be written in the following form:

$$\overline{E}_s = \sum_i \overline{E}_{si} P_{si} + \int E P_{sc}(E) dE \qquad (1)$$

This assumes that a discrete spectrum and a continuum spectrum are both present; obviously one or other may be missing (i.e. FC or FD may be zero).

For a discrete spectrum, the energies to be used in the summation may be simply the discrete energies, E_{si}, given in the file. For some decay modes, however, they may be derived values that make allowance for effects such as neutrino energy or recoil energy. For this reason we use the symbol $\overline{E}_{si}$ to denote the energies used in this check. Special cases are discussed in more detail in Section 4

3.2 Check 2: Average decay energy for "β", "γ" and "α"

For each of the three broad classes of radiation ("β", "γ" and "α"), the values of ER_{AV} given for the radiation types within this class should sum to the values $E_{"\beta"}$, $E_{"\gamma"}$ and $E_{"\alpha"}$ given in the first part of the file:

$$\overline{E}_{"x"} = \sum_{s \in "x"} \overline{E}_s \qquad (x = \beta, \gamma, \alpha) \qquad (2)$$

where "β" includes β^-, β^+ and e^-
"γ" includes γ and x
"α" includes α, n, SF and p

Measures required to allow for annihilation radiation, internal bremsstrahlung and recoil energy are discussed in Section 4.

3.3 Check 3: Q value

A Q value is given for each possible decay mode of the nuclide. An "Effective Q-Value" for decay of the nuclide can be obtained by summing these values weighted by the branching fractions. It should be possible to reproduce the same value with a "Calculated Q-Value" obtained by summing energies from the sections giving data on the spectra of the various types of emitted radiation. This check may be written as follows:

$$\sum_r Q_r B_r = \sum_s \left(\sum_i \tilde{E}_{si} P_{si} + \int E P_{sc}(E) dE \right) \qquad (3)$$

The discrete energies used for the Calculated Q Value on the right hand side may be simply the energies given in the file, but in some cases (discussed in Section 4) alterations may be necessary. The *tilde* is used on the symbol for this reason. These energies may be different from those used in Check 1, since the Q value check must include the neutrino energy.

4. SPECIAL PROBLEMS

4.1 β^- decay

4.1.1 Average beta energy

The energy spectrum for β^- radiation is normally given as a discrete spectrum. The discrete energies are the end point or transition energies, which include the antineutrino energy. This is the correct energy to use when checking the Q value, so we should set $\tilde{E}_{si} = E_{si}$ in Check 3. For Check 1, however, we require a β^- energy, $\overline{E}_{si}$, which excludes the antineutrino energy. This information is not provided explicitly in an ENDF-6 file. If this check is to be performed, the mean β^- energy corresponding to the given end point energy must be calculated from decay theory.

4.1.2 Internal bremsstrahlung

A small part of the available decay energy is emitted as a gamma-ray from internal bremsstrahlung. This energy is not shown explicitly in an ENDF-6 file. In files produced using COGEND, it forms part of the average electromagnetic radiation energy, $E_{"\gamma"}$, but it is not included in the ER_{AV} value for any emitted radiation type (STYP), nor does it appear in the spectrum data for any STYP. Thus Check 2, which compares the sum of the appropriate ER_{AV} values with the $E_{"\gamma"}$ value, will indicate an error unless the internal bremsstrahlung energy is calculated by the checking code and added to the sum. The ENDF-6 format guide does not define any specific procedure for internal bremsstrahlung, and it is possible that files produced by other methods may treat it differently or not treat it at all. This point will therefore require further investigation.

4.2 Electron capture / β^+ decay

4.2.1 Average beta energy

The situation described in the Section 4.1.1 applies similarly to the neutrino energy accompanying β^+ emission. To perform Check 1, it is necessary to calculate the mean β^+ energy corresponding to the given end point energy.

4.2.2 Internal bremsstrahlung

The measures required to allow for internal bremsstrahlung are similar to those described in Section 4.1.2.

4.2.3 Electron capture

There is a difficulty in formulating the Q value check (Check 3) in the case of electron capture. For electron capture, the discrete energies, E_{si}, are equal to the neutrino energy plus the binding energy of the captured orbital electron (plus internal bremsstrahlung energy). An amount of energy equal to this binding energy is emitted in the form of X-rays and/or Auger electrons in filling the vacancy created by the captured electron (and the further chain of vacancies created in this process). These X-ray and electron energies are defined explicitly in

the subsections for STYP 9 and 8. Hence, they will be counted twice if Equation (3) is used with $\tilde{E}_{si} = E_{si}$.

This problem could be resolved by using the equation applied by OKDK, i.e.

$$\text{Calculated Q Value (E.C.)} = \sum_i E_{2,i} P_{2,i} + \sum_i E_{0,i} P_{0,i} (1 + R_{ICC,i}) \qquad (4)$$

where s=2 in the first term denotes electron capture, s=0 in the second term denotes gamma-rays, and $R_{ICC,i}$ is the Total Internal Conversion Coefficient associated with each gamma-ray *i*. This formula avoids the problem of double counting by not using the X-ray (STYP 9) and electron (STYP 8) data, but it means that these data are not checked with respect to their contribution to the total Q value.

Alternatively, the $\tilde{E}_{2,i}$ values in Equation (3) could be set so that they exclude the electron binding energy. However, the required information is not given in the evaluated files, and would have to be calculated. It is calculated by COGEND, so the relevant coding could be extracted and added to the checking code.

4.2.4 Positron annihilation energy

β^+ emission is only possible if the available decay energy is greater than 1.022 MeV. This is the energy equivalent of a negatron/positron pair, and it appears shortly after the decay in the form of the gamma-rays produced in the annihilation of the β^+ particle. Thus the discrete energy in an ENDF-6 file is equal to the sum of the β^+ energy, the neutrino energy and the annihilation energy (and the internal bremsstrahlung energy). However, the annihilation energy is also included in the data given for STYP 9. In setting up the Q value check, care must therefore be taken not to count the annihilation energy twice. This may be achieved by subtracting 1.022 MeV from $E_{2,i}$ in order to set the $\tilde{E}_{2,i}$ value used in the Q value check (Check 3), taking care to do this only for the β^+ emissions and not for the electron capture. The ENDF-6 file provides all the information needed to do this.

For the average energy check (Check 1), the calculation of the average β^+ energy described in Section 4.2.1 must take account of the reduction of 1.022 MeV in the available energy. Apart from this, there should be no further problems with Checks 1 and 2 since the annihilation energy is included in the data for STYP 9 and will therefore appear in the electromagnetic ("γ") total.

4.3 α decay

In α decay, the recoil energy of the daughter product is significant, and must be included in all the checks. The energy spectrum for α radiation is normally given as a discrete spectrum. The discrete energies are the energies of the alpha particles only, but the ENDF-6 format guide specifies that the ER_{AV} value given for this radiation type should include the recoil energy of the daughter. This means that the file provides the appropriate energy for use in Check 2, but that the recoil energy should be added to the discrete energies to provide the values of $\bar{E}_{si}$ and $\tilde{E}_{si}$ used in Checks 1 and 3. The recoil energy is given by

$$E_R = \frac{M_\alpha}{M_R} \left| E_\alpha \right.$$

where M_α is the mass of an alpha particle and M_R is the mass of the daughter. Unfortunately, the mass of the daughter is not given in the file. As an interim measure, OKDK circumvented this problem in the Q Value check (Check 3) by using ER_{AV} in place of the sum over the discrete alpha energies. This allows an overall check to be completed but it does not check the individual alpha energies and their intensities. The alternative is to obtain the mass of the daughter by reading an evaluated data file for the daughter or by using mass tables.

4.4 Other decay modes

For isomeric transition, no special problems are expected in setting up the checks.

For neutron emission, spontaneous fission, proton emission and for multi-particle decays, it is expected that further problems may arise. These have not been examined in any detail in this review but, for example, past work has shown the need to take account of recoil energy in the β^--α decay of ^{17}N. Care must be taken to identify the daughter and its energy state. However, this detail is not present in either OKDK or FIZCON, so its study can be left to the development stages of this work.

5. OKDK

As it stands, the prototype OKDK code performs the three checks outlined in Section 3, but it is limited in the types of decay data that it can handle properly. Some of the main features of the code are listed below, including those areas where it is currently limited and would require further development.

a) **β^- decay:** It does not separate the beta energy, the antineutrino energy and the internal bremsstrahlung energy, so Checks 1 and 2 cannot be performed properly. Check 3 is performed using a formula for the Calculated Q Value similar to that used for electron capture / β^+ decay (Equation (4)). This should work correctly, but it does not check the spectrum data for the electrons (STYP 8) and X-rays (STYP 9).

b) **Electron capture / β^+ decay:** It does not separate the beta energy, the neutrino energy, the annihilation energy (when necessary) and the internal bremsstrahlung energy, so Checks 1 and 2 cannot be performed properly. Check 3 is performed using the formula for the Calculated Q Value given in Equation (4). This avoids the problem of double counting for electron capture described in Section 4.2.3, and should work correctly, but it does not check the spectrum data for the electrons (STYP 8) and X-rays (STYP 9).

c) **α decay:** It cannot perform Check 1 properly for the alpha particle energy because the mass of the daughter is not available for calculating the recoil energy. For the Q value check, Check 3, it circumvents this problem by using the ER_{AV} value in place of the sum of the discrete energies.

d) **Other decay modes:** It should be working correctly for Isomeric Transition, but no special measures have been included to ensure correct treatment of other decay modes such as neutron emission, spontaneous fission, proton emission and multi-particle decay.

e) **Types of spectrum:** It handles discrete spectra but not continuum spectra.

f) **Output:** It does not set any tolerances, but simply prints out the fractional differences for all the checks. It delivers an annotated listing of every evaluation. This feature is available in the LISTEF code [7], and the application of this level of print when checking a complete library is probably undesirable. However, an output of this type is needed in order to study the fractional differences identified by the code.

6. FIZCON

The latest version of FIZCON available from the NEA Data Bank is Version 6.11, dated April 1998. This has been obtained from the Data Bank and installed at Winfrith. Its capabilities for checking decay data have been reviewed by examining the Fortran source code and by running it for some decay data files from JEF2.

The decay data checking is performed by the subroutine CHK457. The checks include the three specified in Section 3. The main features are listed below.

a) **β^- decay:** It incorporates a subroutine (AVG) which, given the end point energy from the file, calculates the mean β^- energy. It is thus able to separate the beta and neutrino energies. This allows Check 1 to be performed properly, provided that the method used by subroutine AVG to calculate the mean β^- energy can be regarded as a reference against which the method used to produce the evaluated file can be tested. There is no allowance for the internal bremsstrahlung energy in Check 2 for the electromagnetic radiations. Check 3 should work correctly.

b) **Electron capture / β^+ decay:** Again, it uses subroutine AVG to separate the beta energy and the neutrino energy. It also makes allowance for the fact that the discrete energy values in the file include the energy equivalent of a positron/negatron pair. The average energy checks 1 and 2 should therefore be correct, apart from the effect of internal bremsstrahlung in Check 2 for the electromagnetic radiations. For the Q Value check (Check 3), however, there are no measures to avoid the problem of double counting for electron capture described in Section 4.2.3. As a result, spurious error messages may be produced. An example, the decay of Cr51, is shown in Appendix A.

c) **α decay:** In Checks 1 and 3, there appears to be no allowance for the fact that the discrete energies in the file do not include the recoil energy of the daughter.

d) **Other decay modes:** It should work correctly for Isomeric Transition. There appear to be no special measures connected with other decay modes such as neutron emission, spontaneous fission, proton emission and multi-particle decay, but the need for such measures has not been examined in any detail in this review.

e) **Types of spectrum:** It handles both discrete spectra and continuum spectra.

f) **Output:** It prints a failure message if the difference is outside the tolerance; otherwise there is no output. The failure messages are brief, and do not identify very clearly the problem that has been found. Coupled with the lack of documentation, this causes significant work to understand problems. The code uses the uncertainties given in the file as tolerances for the checks. It appears that the use of the uncertainties could lead to some rather generous tolerances, since it does not allow for possible correlations. For

example, a run for U235 did not flag the discrepancy associated with the recoil energy of the α-decay daughter (see item c), whereas a run for Sm146 (with a larger discrepancy and smaller uncertainties) did produce failure messages for Checks 1 and 3.

g) **Other checks:** FIZCON applies a number of other checks to the decay data:

- Values are within expected bounds, where these are known.
- Uncertainties are less than 100%.
- Branching ratios add up to 1.0.
- Discrete energies and maximum continuum energies are less than the Q value for the relevant decay mode.
- Spin and parity values are valid.

7. DISCUSSION

Both OKDK and FIZCON contain the framework for performing the three main checks required for decay data, as outlined in Section 3. Both codes would need some further development to provide fully satisfactory checking covering all the required decay modes. From this review it appears that FIZCON already meets more of the requirements, notably the calculation of average beta energies and the treatment of continuum spectra. In practice, however, there would probably be no great difference in the overall amount of work needed.

The Fortran source of both codes appears to be well written, simply structured and adequately commented. Only limited documentation exists for OKDK, since this has so far been developed only as a prototype version. The documentation issued with the FIZCON code package gives information on how to run the code, but it gives only the briefest outline of the checks that are performed.

FIZCON is a comprehensive checking code for all types of data in the ENDF-6 format. It is already used extensively on evaluations produced for the JEF project. Other codes in the same ENDF Utility Package [7] from Brookhaven are also used. For example, CHECKR checks that the evaluated file is correctly structured in the ENDF-6 format. It is often difficult to correct errors by direct examination of the complex ENDF-6 format evaluated files, and the Brookhaven code LISTEF is used to obtain an annotated listing that allows the data to be reviewed much more quickly. It seems better to avoid introducing a further code, *viz.* OKDK, into the checking procedure if FIZCON can perform the required task.

If a modified version of FIZCON is to be produced, there can be no guarantee that the authors of the code at Brookhaven will wish to incorporate the changes in future versions that they issue. However, details of any changes should be sent to the authors for their comments, and a procedure would need to be set up for keeping the modified version up to date with any new versions issued from Brookhaven.

The development of OKDK provided an important stage in understanding decay data and in testing equations in FIZCON. Without the prototype OKDK, and owing to the limited documentation on FIZCON, a new user of FIZCON might be unaware of the current limitations in its decay data checking.

8. CONCLUSIONS

It is recommended that FIZCON be adopted as the code for checking the validity of the decay data files for the JEF project, with the necessary code developments being made to meet the outstanding requirements. Clear detailed documentation needs to be provided for the developed code.

9. REFERENCES

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APPENDIX A
DETAILED BREAKDOWN AND FIZCON RESULTS FOR CR51 DECAY

This appendix shows an example of the type of problem that can arise in setting up a checking procedure. Cr51 decays by electron capture. FIZCON has been run for three Cr51 evaluated decay data files: ENDF/B-VI (Rev. 4), JEF2.2 and UKPADD6. In each case, a "total energy release sumup failure" was reported. This is the Q Value check - Check 3. The output from the UKPADD6 case is shown below.

```
 PROGRAM FIZCON VERSION 6.11

 Input File Specification-----------------------UKPADD6CR51
 Check the Entire Tape
 Sum Up Tests will be Performed
 Deviant Point Check will be Performed
 Consecutive Equal Value Check will be Performed
1
    CHECK MATERIAL 2428
                              (NO ERRORS DETECTED IN SECTIONS WITHOUT COMMENTS)

 ------------------------------------------------------------------------------
 FILE  1
    SECTION 451
       24-CR- 51 WTC        EVAL-AUG89 A L NICHOLS
                            DIST-OCT92                      921018
      ----UKPADD-6          MATERIAL 2428
      -----RADIOACTIVE DECAY DATA
      ------ENDF-6 FORMAT

 ------------------------------------------------------------------------------
 FILE  8
    SECTION 457
      TOTAL ENERGY RELEASE SUMUP FAILURE              SEQUENCE NUMBER    56
          WHOLE= 7.51300E+05  SUM= 7.56202E+05
```

"WHOLE" is the Effective Q Value and "SUM" is the calculated Q Value. The following table shows how this calculated Q Value is obtained.

diation type	**Normalising factor**	**Energy (keV)**	**Relative intensity**	**Calculated Q Value (FIZCON method)**	**Calculated Q Value (OKDK method)**
Gamma-ray (STYP 0)	0.0986	320.084	1.0	31.56028	(Internal conversion coefficient = 0.00169) 31.61362
Electron capture (STYP 2)	1.0	431.2 751.3	0.0988 0.9012	719.6741	719.6741
Electrons (STYP 8)	1.0	0.0293 0.4500 4.522 314.619 319.571 320.055	3.12809 1.50038 0.671099 1.50858E-4 1.3311E-5 2.465E-6	3.854039	-
X-rays (STYP 9)	1.0	4.94464 4.9522 5.4300	0.0657352 0.130427 0.0263462	1.113997	-
TOTAL				756.2024	751.2877
Effective Q Value from file = 751.3 keV					

The Calculated Q Value obtained by the FIZCON method is too high because the binding energy of the captured electron forms part of each of the discrete energies given for electron capture (STYP 2) but it also forms part of the energy given in the electron (STYP 8) and X-ray (STYP 9) sections.

The Calculated Q value obtained by the OKDK method agrees with the Effective Q Value. This result is achieved by excluding the electron and X-ray (STYP 8 and 9) data from the summation, and making use of the internal conversion coefficient to ensure that account is taken of those electrons and X-rays that are associated with internal conversion. Thus the double counting problem is avoided, but the electron and X-ray (STYP 8 and 9) data are not checked.