Fission Yield Data Evaluation System FYDES

Liu Tingjin
(China Nuclear Data Center, CIAE)

Introduction

The retrieval and processing for fission yield data evaluation are quite complicated, and differ from the general complete set of neutron data evaluation in the following aspects:

1) The data in EXFOR file could be under the heading "ELEM/MASS";
2) There are more relative ratio measured data, and the data could be R-value;
3) More data need to be corrected for standard yield, gamma intensity and fission cross section and calculated from ratio or R-value;
4) For most cases, the dependence of yield on neutron energy seems linear.

Taking account of above features of fission yield data, to do the fission yield data evaluation conveniently, a fission yield data evaluation system FYDES has been developed for last two years.

1 Outline of the System

The main diagram of FYDES is shown in Fig.1.

The data are retrieved from the EXFOR Master Library with EXFOR Library Management System according to the reactions, producing EXFOR data and their index files *.EXFOR and *.INDEX, and sometimes also with code NEXFOR according to the entry (subentry) number.

The data tables with columns less than six are firstly standardized by using code FORM, producing standard data file *.FOM and then taken out with code FYRET, producing data file *.TAB. The data tables with columns more than six are firstly taken out with code FYRETD and then standardized by using code FYDEXCH. The necessary corrections are made by means of codes FYCRECT (less six columns), or FYCRECTD (more than six columns), producing data file *.CRE and FYCRECT1 (second time if needed). Then the data are retrieved by code FYRET1 according to product nuclides, producing data file *.DAT.

If there are some measurements at same energy point, they are averaged by using code AVERAG and if there are some fission yield and their ratio measurements at the same time, they are simultaneously evaluated with code ZOTT, producing data file *.PRO.

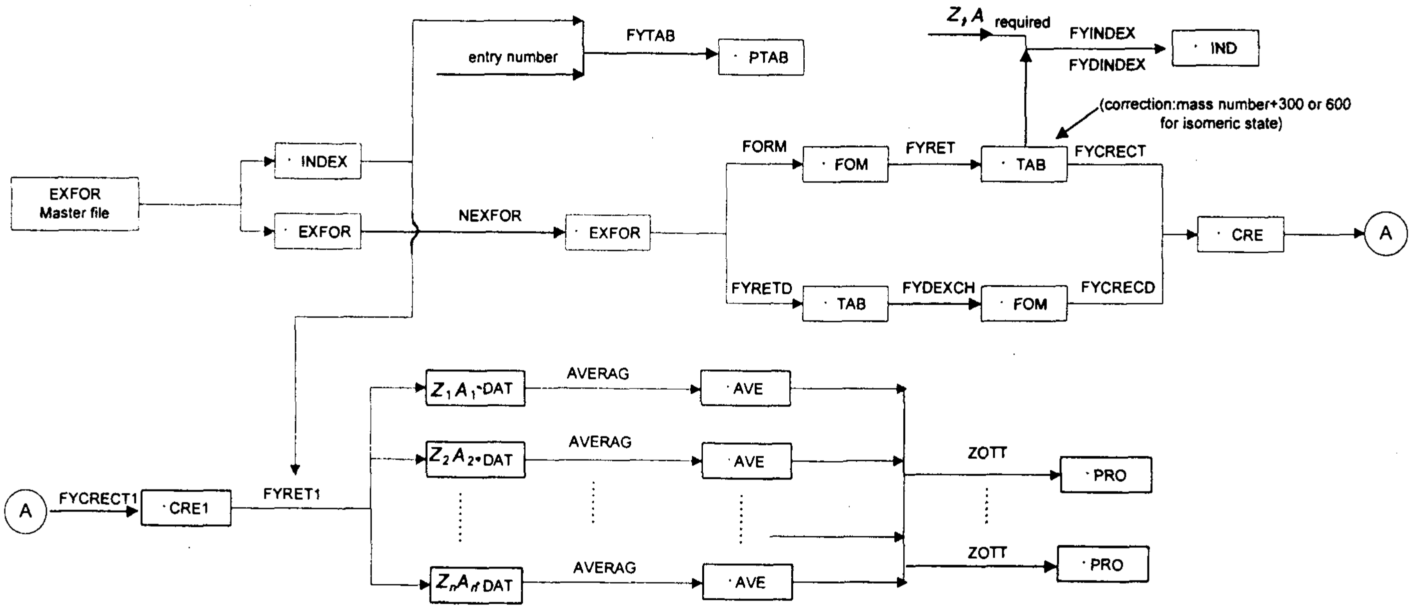

Fig.1 The main diagram of fission product yield data processing

If it is needed to give out the dependence of the yield on neutron energy, the data can be fitted by using code LIFIT with options of $y = aE+b$ or $y = y * \exp(aE)$. If the linear function could not fit the data well, then the data can be fitted with code SPF for any shape curve.

There are also some auxiliary codes FYINDEX, FYDINDEX for making index list of the product nuclides in each EXFOR subentry and FYTAB to make index table for abstract recording.

2 Data Retrieval and Data Table Standardization

The FY data can be retrieved according to the target, incident neutron energy and products by using EXFOR retrieval system. However when a product is given under the heading "ELEM/MASS", it could not be found.

To solve this problem, some supplementary programs were developed and they can be used following the retrieving by EXFOR system "RETREV", "COFFEE-CS" in the option "P" and default to the reaction field 4 (reaction product).

1) FORM[1] Exchange the column position and make the data table standardization:

Column	1	2	3	4	5	6
	Z	A	DATA	DATA-ERR		

Also make the "DATA-ERR" become absolute error.

2) FYRET Take the data table from each subentry in EXFOR data file.

3) FYRET1 Retrieve FY data according to the special Z and A, and read the reaction quantity, neutron energy, EXFOR entry number from the index file and write into the file.

If the quantities in a "HEADING" are over six (take two rows), instead of above, the following programs can be used:

4) FYRETD take out the data table.

5) FYEXC Exchange the column position and make the data table standardization.

6) FYRET1D Retrieve FY data according to Z and A.

The following should be noted, when use these codes:

(a) If the FY data are given for more than one energy point in an entry, the energy given in the retrieved data file is only maximum one.

(b) Due to there is no other function (only exchanging column position), the error in the file processed by FYRET1D may be relative or only statistical one and must be treated by following codes FYCRECT and FYCRECT1.

3 Data Correction, Codes FYCRECT and FYCRECT1

Table 1 Some examples of running code FYCRECT and FYCRECT1

13097003	11	(FY CALCULATED FROM Ro, ERR 7% GIVEN)			
ELEMENT	MASS	FY DATA	FY ERR		
NO−DIM	NO−DIM	PC/FIS	PC/FIS		
36.0	93.0	0.075	0.010		
36.0	94.0	1.500E−02	5.000E−03		
36.0	97.0	0.000E+00	0.000E+00		
37.0	91.0	0.930	0.050		
54.0	138.0	9.570E−01	2.000E−03		
55.0	139.0	9.880E−01	3.000E−03		
55.0	140.0	0.934	0.026		
55.0	141.0	4.245	0.297		
56.0	141.0	9.964E−01	1.700E−03		
56.0	142.0	9.810E−01	5.000E−03		
57.0	143.0	9.956E−01	3.000E−03		
13116002	6	(FY CORRECTED FOR GAMMA INTENSITY)			
ELEMENT	MASS	FY CREC	ERR CREC	FY ORIG	Irn/Ir0
NO−DIM	NO−DIM	PC/FIS	PC/FIS	PC/FIS	NO−DIM
36.0	85.0	3.989E−03	0.000E+00	3.980E−03	9.977E−01
63.0	156.0	7.247E−04	0.000E+00	5.140E−04	7.092E−01
65.0	161.0	4.932E−05	0.000E+00	4.090E−05	8.293E−01
36.0	85.0	4.009E−03	0.000E+00	4.000E−03	9.977E−01
63.0	156.0	7.543E−04	0.000E+00	5.350E−04	7.092E−01
65.0	161.0	5.282E−05	0.000E+00	4.380E−05	8.293E−01
13174002	3	(FY CORRECTED FOR GAMMA INTENSITY)			
ELEMENT	MASS	FY CREC	ERR CREC	FY ORIG	Irn/Ir0
NO−DIM	NO−DIM	PC/FIS	PC/FIS	PC/FIS	NO−DIM
36.0	85.0	3.197E−03	3.000E−05	3.190E−03	9.977E−01
63.0	156.0	2.975E−04	2.000E−06	2.110E−04	7.092E−01
65.0	161.0	2.894E−06	1.300E−07	2.400E−06	8.293E−01
13202002	3	(FY CALCULATED FROM RATIO AND STANDARD)			
ELEMENT	MASS	FY DATA	ERR CALC	REL ERR	
NO−DIM	NO−DIM	PC/FIS	PC/FIS	PER−CENT	
36.0	84.0	9.963E−01	1.993E−02	2.00	
36.0	85.0	2.890E−01	5.780E−03	2.00	
36.0	86.0	1.948E+00	3.896E−02	2.00	
		(FY ERROR CALCULATED FROM GIVEN *c*%)			
13207002	7	(FY CALCULATED FROM RATIO AND STANDARD)			
ELEMENT	MASS	FY DATA	ERR CALC	REL ERR	
NO−DIM	NO−DIM	PC/FIS	PC/FIS	PER−CENT	
37.0	89.0	5.130E+00	7.695E−02	1.50	
37.0	90.0	4.628E+00	6.942E−02	1.50	
37.0	91.0	5.576E+00	8.364E−02	1.50	
37.0	92.0	5.075E+00	7.612E−02	1.50	
37.0	93.0	3.904E+00	5.856E−02	1.50	
37.0	94.0	1.952E+00	2.928E−02	1.50	
37.0	95.0	8.360E−01	1.254E−02	1.50	
		(FY ERROR CALCULATED FROM GIVEN *c*%)			

The data were corrected by using codes FYCRECT and FYCRECT1, The functions and options for these codes are as follows:

1) Calculate absolute fission yield and its error from given ratio, standard and their errors;

2) Calculate ratio and its error from given R-value, standard fission yields and their errors at energy points to be measured and thermal;

3) Calculate ratio and its error from given fission yield, standard and their errors used;

4) Correct for standard fission yield and fission cross section;

5) Correct for gamma intensity used;

6) Calculate absolute error from given relative error;

7) Calculate absolute error from given relative error c% for the errors less than c%;

8) Calculate absolute error from given relative error in 4th column of the Table;

9) Calculate absolute total error from given absolute error1 and error2 in the Table;

10) Calculate absolute error from given absolute error1 in the data table and given additional relative error 2 (all the same).

The functions of two codes are the same, but FYCRECT1 is interfaced with FYCRECT and keeps the information written by FYCRECT.

An example of data correction is shown in Table 1, which was taken from the reference fission yield data evaluation.

4 Data Averaging, Code AVERAG

The data are averaged with code AVERAG. The mean with weight and its external error are calculated.

$$\overline{Y}_{w} = \sum_{i}^{N} W_i Y_i \Big/ \sum_{i}^{N} W_\varepsilon$$

$$\Delta \overline{Y}_{ex} = \begin{cases} \varepsilon \Delta \overline{Y}_{in} & (\varepsilon \geq 1) \\ \Delta \overline{Y}_{in} & (\varepsilon < 1) \end{cases}$$

$$\varepsilon = \left(\frac{1}{N-1} \sum_{i=1}^{N} W_i (Y_i - \overline{Y}_w)^2 \right)^{\frac{1}{2}} = \left(\chi^2_{red}\right)^{\frac{1}{2}}$$

$$\Delta \overline{Y}_{in} = \left(\frac{1}{W} \right)^{\frac{1}{2}}$$

Where $W_i = \Delta Y_i^2$ $\quad W = \sum_{i=1}^{N} W_i$

It can be seen that the errors given for each set of data and the discrepancy between the data sets are taken into account. In general case, the mean with weight and its external error are recommended.

The reduced χ^2 and internal error, and their arithmetical mean and its error are also calculated for reference.

An example of using AVERAG is given in Table 2.

Table 2 An example of running code AVERAG

^{235}U CUMUL FY DATA FOR FP $Z = 56$ $A = 140.0$			
Input Data			
(FY—Fission yield, DY(A)—Absolute error of FY, DY(%)—Relative error of FY)			
	FIS Y	DY(A)	DY(%)
12771005	5.8100E+00	3.4860E−01	6.0000E+00
13383002	6.3200E+00	9.4800E−01	1.5000E+01
13398002	6.1500E+00	9.2300E−01	1.5008E+01
13486002	6.2000E+00	6.2000E−01	1.0000E+01
21483002	6.3600E+00	4.5000E−01	7.0755E+00
22054002	6.2740E+00	9.0000E−02	1.4345E+00
30495002	6.2720E+00	3.1400E−01	5.0064E+00
32635003	6.2000E+00	3.9000E−01	6.2903E+00
32638003	6.2680E+00	1.4100E−01	2.2495E+00

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Calculated Average Fission Yield WY with Weight
(WY—Average value with weight, EY(A)—External absolute error of WY, EY(%)—External relative error of WY, EY(I), EY(%)—Internal absolute and relative error of YP)

WY	6.2525
EY(A)	0.0692
EY(%)	1.1076
EY(I)	0.0692
EY(%)	1.1076
EPS	1.00000

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Calculated Arithmetic Average Value AY

AY	6.2060
EY(A)	0.0539
EY(%)	0.8693

5 Simultaneous Evaluation, Code ZOTT

Simultaneous evaluation is completed with code ZOTT[2], taking account of measured absolute fission yields, their ratios and the measured errors as well as their correlations, making them consistent. Using partitioned least squares method, the

Table 3 An example of running code ZOTT

1) Input Data File			
NY, NB, IPRINT, ILOG, ICOV			
7 3 0 1 1			
COMBINED Y−VECTOR FOR ^{147,149,151,152}Sm. AT THERMAL			
2.1127 1.0212 0.40428 0.24893 2.106 0.3982 0.25063			
TOTAL ERROR AND CORRELATIVE ERROR			
0.02535 0.04801 0.004852 0.087446 0.03159 0.005973			
0.002899			
0.0			
SENSITIVITY (= R)			
1 −1 0 0			
0 −1 1 0			
0 −1 0 1			
2) Output Result(Part)			
COMBINED Y−VECTOR FOR ^{147,149,151,152}Sm			
2.112700E+00	1.021200E+00	4.042800E−01	2.489300E−01
2.106000E+00	3.982000E−01	2.506300E−01	
(the intermediate results were omitted)			
ADJUSTED Y'			
2.118375E+00	1.010102E+00	4.034757E−01	2.531572E−01
2.097189E+00	3.994406E−01	2.506254E−01	
APPROXIMATE RELCOV(Y') BY COV LN(Y') = COV(THETA')			
S.D.(Y')			
2.258691E−02	1.317217E−02	4.302739E−03	4.408931E−03
2.577328E−02	4.908932E−03	2.897379E−03	
ADJUSTED CORRELATION MATRIX			
1.000000E+00	4.772272E−01	2.277696E−01	3.569470E−01
3.612147E−01	−3.087407E−01	−5.830039E−04	
4.772272E−01	1.000000E+00	4.772781E−01	7.479621E−01
−6.470671E−01	−6.469486E−01	−1.221651E−03	
2.277696E−01	4.772781E−01	1.000000E+00	3.569851E−01
−3.088302E−01	3.613055E−01	−5.830661E−04	
3.569470E−01	7.479621E−01	3.569851E−01	1.000000E+00
−4.839805E−01	−4.838919E−01	6.628853E−01	
3.612147E−01	−6.470671E−01	−3.088302E−01	−4.839805E−01
1.000000E+00	4.186181E−01	7.904885E−04	
−3.087407E−01	−6.469486E−01	3.613055E−01	−4.838919E−01
4.186181E−01	1.000000E+00	7.903437E−04	
−5.830039E−04	−1.221651E−03	−5.830661E−04	6.628853E−01
7.904885E−04	7.903437E−04	1.000000E+00	

"microscopic" or "elementary" and "macroscopic" or "duplicated" quantities, For example, partial and total cross section, fission yield and its ratio etc., are adjusted to get the optimum values with minimum variance derivation. Using ZOTT, not only the adjusted fission yields and ratios, but also their covariance matrix can be calculated.

The key point for using ZOTT is to construct the sensitive matrix, which describe the relationship among the quantities in the input vector. From the application point of view, it can be keep in mind that the column number of matrix is equal to the number of 'elementary' or 'microscopic' quantities (absolute fission yields at present case), and row number is equal to the number of the 'duplicated or 'macroscopic' quantities (ratios at present case). Each element is equal to 1, −1, or 0, representing the numerator, denominator, or no relation in the ratio of the corresponding 'elemental' quantities, for example, if the first ratio $R_1 = FY_2/FY_3$, the elements at the first row of the matrix are equal to 0, 1, −1 respectively, if $R_2 = FY_3 / FY_1$, the elements in the second row are −1, 0, 1 respectively.

An example of using ZOTT is given in Table 3.

6 Data Fit Programs LIFIT and SPF

The data can be fitted with linear function by using code LIFIT with options for FY = $aE+b$ or ln(FY) = $aE+b$. By means of minimum squares method, the optimum fit coefficients:

$$a = 1/c(c_{22}A_1 - c_{12}A_2)$$
$$b = 1/c(c_{11}A_2 - c_{21}A_1)$$

Were

$$c = c_{11}c_{22} - c_{12}c_{21}$$

$$c_{11} = \sum_i W_i E_i^2 \qquad c_{12} = \sum_i W_i E_i$$

$$c_{21} = c_{12} \qquad c_{22} = \sum_i W_i$$

$$A_1 = \sum_i W_i Y_i E_i \qquad A_2 = \sum_i W_i Y_i$$

For the fitting with $y = y_0 e^{aE}$, let

$$y' = \ln(y) = aE + \ln(y_0) = aE + b$$

And in this case

$$\Delta y' = \Delta y / y$$

so, the coefficients a and b can be calculated according to above formulas, and then

$$y = e^{y'}$$

The reduced χ^2 is calculated

$$\chi^2 = \frac{1}{N} - 2\sum_{i=1}^{N}(Y_i - \hat{Y})/\Delta Y_i^2$$

which express the fit merit.

An example of LIFIT is given in Table 4 and Fig.2

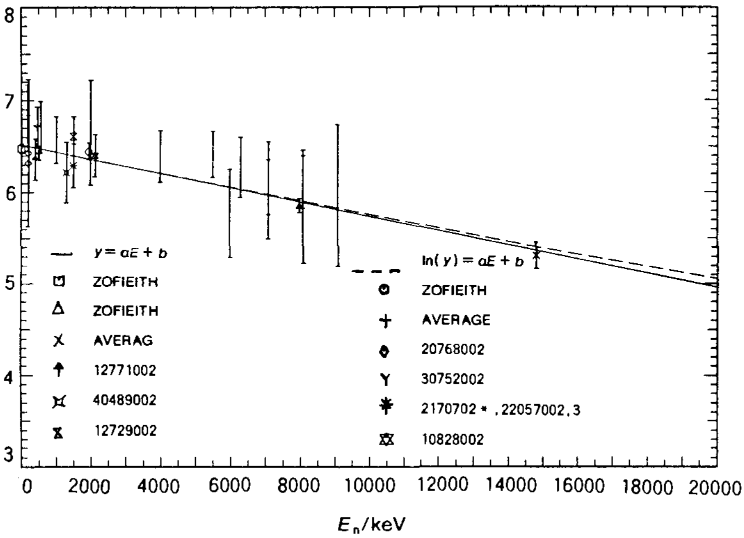

Fig.2 $^{235}U(n,f)^{95}Zr$ cumulative fission yield

Table 4 An example of running code LIFIT

1) Input File		
26	5	1
2.5300E−02	6.4791E+00	5.0450E−02
1.9500E+06	6.4431E+00	9.3610E−02
8.0000E+06	5.8503E+00	7.6130E−02
5.0000E+05	6.4301E+00	7.5500E−02
1.4800E+07	5.3062E+00	1.4480E−01
2.0000E+05	6.3200E+00	5.2000E−01
2.0000E+05	6.4300E+00	8.0000E−01
4.0000E+05	6.3600E+00	2.2430E−01
4.5000E+05	6.7100E+00	2.2000E−01
1.3000E+06	6.2170E+00	3.2800E−01
1.5000E+06	6.2900E+00	2.4000E−01
1.5000E+06	6.6100E+00	2.1000E−01
2.1300E+06	6.4000E+00	2.3000E−01
1.7000E+05	6.8100E+00	3.6000E−01
5.5000E+05	6.7100E+00	2.8000E−01
1.0000E+06	6.5700E+00	2.5000E−01
2.0000E+06	6.6500E+00	5.7000E−01

26	5	1
4.0000E+06	6.3900E+00	2.8000E−01
5.5000E+06	6.4100E+00	2.5000E−01
6.3000E+06	6.2700E+00	3.3000E−01
7.1000E+06	6.0500E+00	3.0000E−01
8.1000E+06	6.1400E+00	3.2000E−01
6.0000E+06	5.7638E+00	4.8000E−01
7.1000E+06	6.0188E+00	5.3000E−01
8.1000E+06	5.8106E+00	5.9000E−01
9.1000E+06	5.9630E+00	7.7000E−01

2.53E−02   1.95E+06   2.13+06   1.48E+07   2.00E+07

2) Output File

LN(Y)−LINEAR(E)   FIT COEFFICIENTS a & b

($\ln(Y) = aE + b$ or $y = aE + \ln(y_0)$)

−1.2748E−08   1.8751E+00   6.5215E+00

****

FIT VALUES	
2.5300E−02	6.5215E+00
1.9500E+06	6.3614E+00
2.1300E+06	6.3468E+00
1.4800E+07	5.4001E+00
2.0000E+07	5.0538E+00

REDUCED KSE SQARE
4.8481E−01

If the data can not be fitted well by LIFIT, for example $\chi^2 > 2.0$, the data can be fitted with code SPF[3], a general spline fitting program for multi-sets of data with knot optimization and spline order selection. It can be used for any shape curve.

An example of SPF is given in Fig.3

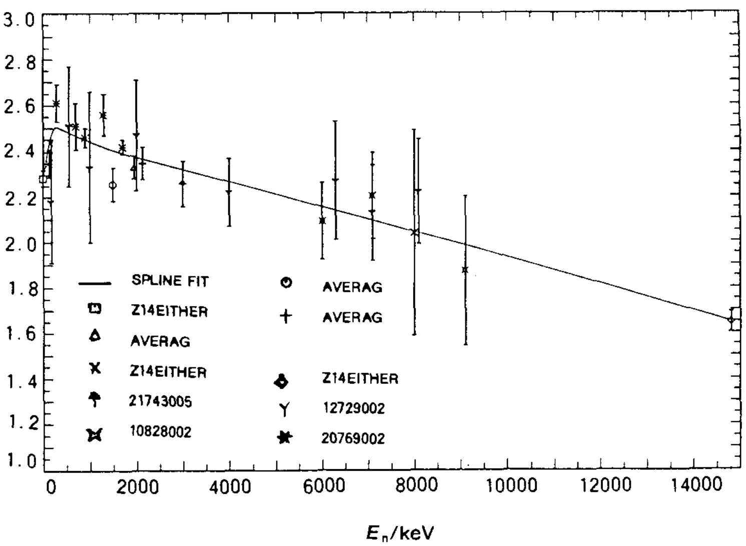

Fig.3 $^{235}U(n,f)^{147}Nd$ cumulative fission yield

References

[1] Liu Tingjin et al, Chinese Jou. of Nucl. Sci. And Eng., 1, 79(1988) (in Chinese)
[2] D. Muir, Nucl. Sci. & Eng., 101, 88(1989)
[3] Liu Tingjin, CNDP, 2, 58(1989)

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Model Calculations for Fission Yields

Shu Nengchuan Liu Tingjin
(China Nuclear Data Center, CIAE)

Abstract

Multi-Gauss model and Zp model are used to calculate fission yields. The results are in well agreement with other data.

Introduction

The long-lived cumulative and chain yields measurements are more numerous and cover a wider range of fission system. In the mean while, they have more accurate data.

Even so, only for a limited set of fission system chain yield are well defined. The common features in this fission system is that in the valley region and at the wings of the chain distribution they have few available experiment data. It is necessary to use calculated data as a reference.

It is even worse for independent fission yields.

Here, Multi-Gauss fitting are used to fitting chain yield, and program Cyi based upon Multi-Gauss and Zp model are used to calculate cumulative and independent fission yields. The results show that most of the data are in agreement with our evaluated data[1~3] and ENDF/B-6 and experimental data.

1 Chain Yield Model and Fitting

The mass distributions of most nuclides' chain yields show some common features. It has a pair of approximately symmetrical peaks with a valley between