GABS v12

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Reference: E. Browne, NIMA **249** (1986) 461, Erratum: NIMA **345** (1994) 215; **1986Br26**

GABS – calculating absolute γ-ray intensities and decay branching ratios derived from decay schemes

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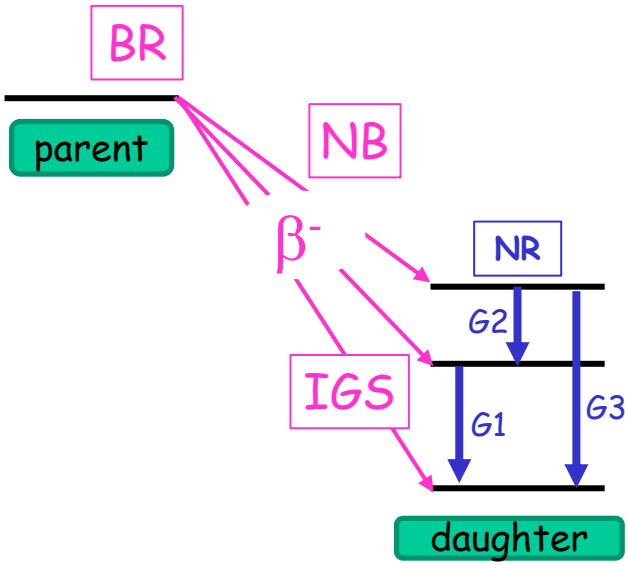
NORMALISATION RECORD:

- **NR**: Multiplier for converting relative photon intensity (RI in the GAMMA record) to photons per 100 decays of the parent through the decay branch
- **BR**: Branching ratio multiplier for converting intensity per 100 decays through this decay branch to intensity per 100 decays of the parent nuclide.
- **NB**: Multiplier for converting relative β and EC intensities (IB in the B- record; IB, IE, TI in the EC record) to intensities per 100 decays through this decay branch.
- **IGS**: fraction (%) of direct β and EC feeding to the g.s.



GABS calculates

- **Single Data Set:** **NR** from **RI**, **CC**, **TI** (if given) , **BR** and **IGS**
- **Multiple Data Set:** **NR and BR** from **RI**, **CC**, **TI** (if given) , and **IGS**

GABS – calculating absolute γ-ray intensities and decay branching ratios derived from decay schemes

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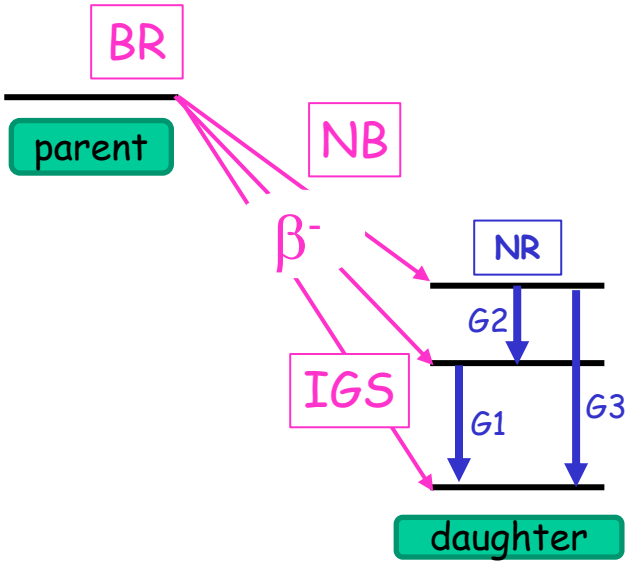
Simple decay scheme



1986Br21 uses G, the fraction of NOT populating the g.s.

GABS: Fractional g.s. feeding, IGS

$$G = \frac{100 - IGS}{100}$$

Definitions:

- Total transition intensity: **TI=RI*(1+CC)**
- Absolute γ-photon intensity: **%IG=NR*BR*RI** per 100 decays
- **NR** and **BR** not independent quantities:

GABS: Calculates **NR** only!

$$TI = RI*(1+CC)$$

$$N = NR*BR$$

$$100 = BR \times [IGS + NR \times \sum_i TI(i)]$$

$$NR = \frac{100 - IGS}{100 \times \sum_i TI(i)}$$

$$\%IG = RI*NR*BR$$

GABS – calculating absolute γ-ray intensities and decay branching ratios derived from decay schemes

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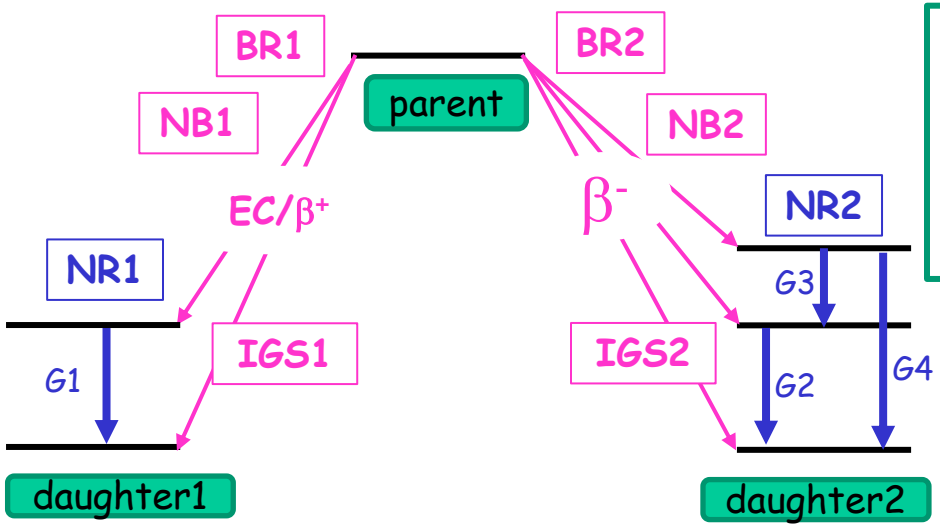
Complex decay scheme with g.s. feeding

Assuming all RI`s are on the same scale or from the same experiment



$$100 = \sum_j BR(j) \times [IGS(j) + NR(j) \times \sum_i TI(i,j)]$$

$$\sum_j BR(j) = 1$$

$$BR(j) \times NR(j) = BR(k) \times NR(k)$$

GABS: Calculates **NR(i) & BR(i)**

Caution: Strong correlation between input parameters

New equations derived for uncertainties in **NR**, **BR** and **%IG**

$$BR(i) = \frac{\frac{100 - IGS(i)}{100} \sum_j TI(j,i)}{\sum_k \frac{100 - IGS(k)}{100} \sum_j TI(j,k)}$$

$$N = NR(i) \times BR(i) = \frac{100}{\sum_k \frac{100 - IGS(k)}{100} \sum_j TI(j,k)}$$

GABS v12

Gamma-rays for normalisation

- Must feed to the ground state
- RI or TI must be given; DRI or DTI could be blank, but $\Sigma(DTI(i)^2) > 0$!
- "X" in column 79
- Gamma-cascade: '*C*' in column 80 on N-record
- **IGS=** on "2 N" record to specify α, β, EC decay branch **feeding to g.s.**; given in %.

New functions added

-F NR and BR will be obtained from a fit (using G`s marked with "X"; normal execution)

-C Calculate **%TI** using **NR** & **BR** from the N-record

-M Mark transitions going to the g.s. with "X" (DRI>0) or "Y" (DRI=0)

Usage gabs -F ENSDF file

gabs ? *for quick help*

GABS v12 – code improvements

- Program logic simplified
- Uncertainties – new analytical formulas
- All variables declared in a single module (F90)
- Variable names changed according to ENSDF manual (RI, TI, NR, CC)
- ENSDF file loaded and kept in memory
- Improved user support (error checking)
- Normalisation Gammas: "CA", "AS", "LT", "LE" "GT" or "GE" not allowed!
- Calculation mode: NR & BR expected to be numeric. Blank BR assumed to be 1.0.
- "CA" or "AS" in the DNR field will make uncertainty in %TI "CA" or "AS". No provisions to handle limits in NR or BR.

gabs ?

Command: gabs ?

========== GABS Version 12 [22-Apr-2020] ==========

Usage with command line arguments:

GABS <Mode> <InputFile>

InputFile ENSDF file, G-rays marked with "X" in column 79
Blank DRI or DTI allowed, but sum[i] DTI(i)**2 should not be zero

Mode to control execution

-F NR and BR (multiple data set only!) will be calculated from
G`s marked with "X" and direct feeding to the ground state (IGS)
Output: report (*.rpt), new ensdf (*.new)

-C Calculate TI using NR and BR from the N-record in the input file
Output: report (*.rpt), new ensdf (*.new)

-M Lists transitions going to the g.s. and RI>0 or TI>0 with
"X" (DRI>0 or DTI>0) or "Y" (blank or limits in DRI or DTI)
Total RI and TI for g.s. transitions also calculated
Output: report (*.rpt), GABS input (*.in)

Calculate NR
Single DS with NO g.s. feeding

gabs –F InpFile

Input file need to be preapred:

```
205PO     205AT EC DECAY         1971JO19,1982KU20,1982KU2104NDS    200404
…………………..
205AT   P 0.0          9/2-            26.9 M            4537      25
205PO DN 0.489      14          0.90    2 1
205PO   N                       0.90    2 1.0
205PO CN NR$ From the decay scheme by assuming SUMOF (TI(GS))=100%. The EC+B+
205PO2CN feeding to the GS is not expected, since it involves a second forbidden
205PO3CN (DJ=2, PI=NO) transition. Note, that normalization factors of 0.31 5
205PO4CN in 1971Jo19 and 0.31 4 in 1982Ku21 imply a significant feeding to
205PO5CN the GS.
…………………..
205PO   L    143.16617 1/2-            310 NS    60                    BM1
205PO   G 143.166    17 2.69   19E2                  1.641                X
205POS G  KC=0.324 5$LC=0.977 14$MC=0.260 4
205POS G  NC=0.0667 10$OC=0.01274 18$PC=0.001163 17
```

NR must be blank

90% EC & 10% α

Blank TI; RI & CC will be used

Calculate NR - gabs -F InpFile
Single DS with NO g.s. feeding

gabs -F InpFile

```
Command:  gabs -F Po205_ec_gabs.in
 ==========  GABS Version 12 [04-Apr-2019]  ==========
Report file:         Po205_ec_gabs.rpt
Loading input file: Po205_ec_gabs.in
  Data set: 205AT EC DECAY

 Calculating new normalization factor * * * * *

Data set: 205AT EC DECAY
Transitions used for normalization:
  205PO  G 143.166    17 2.69    19E2                          1.641                  X
  205PO  G 154.198    12 5.0     4 M1(+E2)    0.22    LE       3.19   7               X
  205PO  G 384.61     14 3.98    20M1+E2      0.87    13       0.173  16              X
  205PO  G 669.41     4  28.1    12E2                          0.01661                X
  205PO  G 719.30     4  100.000  E2                           0.01426                X
  ……..
  205PO  G 3052.0     10 0.200   1                                                    X
  205PO  G 3172.0     15 0.180   1                                                    X

 Normalization: 205AT EC DECAY  NR= 0.589 16  BR= 0.900 20
 E=105.15(10)        %IG=0.111 (16)
 E=123.35(4)         %IG=0.149 (14)
 ……..
 E=154.198(12)       %IG=2.65 (21)      Compare with %IG=2.65(23)
```

ENSDF input routine
Only N and G records are tested

Calibration transitions

Calculation report & list of absolute %IG

Calculate NR
Single DS with NO g.s. feeding

gabs -F InpFile

Report:

```
 * * * * * * GABS Version 12 [04-Apr-2019] Report file  * * * * * *
  Current date: 23:20:59 09-Apr-2019
  ENSDF input file: gabs-test.ens
  Calculating new normalization factor * * * * *
  New ENSDF file:   gabs-test.new

  Data set: 177YB B- DECAY
  Transitions used for normalization:
   177LU  G 150.399   1 354     19E1                          0.512  32          a X
  ……..
  Normalization: 177YB B- DECAY  NR= 0.0508 21  BR= 1.000
   E=150.399(1)        %IG=18.0 (5)      Compare with %IG=18.0(12)
```

Calculated with the "nominal" NR(DNR)

- GABS new NR(DNR) calculated
- 150.399 keV calibration gamma: DNR should not have contribution from GTI(150.399)
- GABS re-calculates DNR and folds in DRI to calculate %DIG

Calculate NR
Single DS with NO g.s. feeding

gabs -F InpFile

New ENSDF file:

```
 177LU    177YB B- DECAY                  1995Ya21                    03NDS     200305
 ……..
177YB  P 0.0             9/2+              1.911 H   3               1397.4    12
177LU  N  0.0508   21           1.0
177LU PN                                                                        6
177LU CN NR$From SUMOF TI[TO 177LU GS]=100-%IB-(GS), where the direct feeding
177LU2CN to the 177LU GS, %IB-(GS)=59.4% 5 (1995Ya21).
177LU3CN Others: 0.044 {I5} from Ice(121|g)=5.25% (1964Jo03) and
177LU4CN |a=2.00 {I4}, 0.039 {I5} from Ice(150|g)=7.0% (1964Jo03) and
177LU4CN |a=0.512 {I32} and 0.044 {I5} from Ice(138|g)=1.5% (1964Jo03) and
177LU5CN |a=1.43 {I3}
 ……..
177LU  G 150.399   1 354     19E1                        0.512  32              a
177LU2 G  %IG=18.0 5
 ……..
```

Old "2 G" cards removed

Calculate NR - gabs -F InpFile
Single DS with g.s. feeding

gabs -F InpFile

Input file:

```
177LU    177YB B- DECAY                    1995Ya21
……….
177YB  P 0.0          9/2+                1.911 H   3                1397.4    12
177LU  N                          1.0
177LU2 N IGS=59.4 5
177LU PN                                                                      6
177LU CN NR$From SUMOF TI[TO 177LU GS]=100-%IB-(GS), where the direct feeding
177LU2CN to the 177LU GS, %IB-(GS)=59.4% 5 (1995Ya21).
177LU3cN Others: 0.044 {I5} from Ice(121|g)=5.25% (1964Jo03) and
177LU4cN |a=2.00 {I4}, 0.039 {I5} from Ice(150|g)=7.0% (1964Jo03) and
177LU4cN |a=0.512 {I32} and 0.044 {I5} from Ice(138|g)=1.5% (1964Jo03) and
177LU5cN |a=1.43 {I3}
……….
```

59.4(5)% direct feeding to GS

Calculate %IG using NR & BR from ENSDF – gabs –C InpFile

gabs –C InpFile

```
Command: gabs -C gabs-test2.in
========== GABS Version 12 [04-Apr-2019] ==========
 Report file:       gabs-test2.rpt
 Loading input file: gabs-test2.in
   Data set: 177YB B- DECAY
     <W> No NB given, assumed NB=1
 Loading input file: gabs-test2.in
   Data set: 177YB B- DECAY
     <W> No NB given, assumed NB=1

 Running in Calculation mode * * * * *
 Output file opened: gabs-test2.new
 Report file:       gabs-test2.rpt

 Data set: 177YB B- DECAY
 Normalization:    NR=0.0508(21)
                   BR=1.0
             N=NR*BR=0.0508(21)

 Calculations completed
```

Calculate %IG using NR & BR from ENSDF

gabs -C InpFile

New ENSDF:

```
177LU    177YB B- DECAY              1995Ya21              03NDS    200305
.....
177LU  G 150.399   1.354    19E1                0.512  32          a
177LU2 G %IG=18.0 12
```

%IG should be 18.0(5)

CAUTION: GABS could overestimate **%DIG** if this transition was used to derive **NR** and **BR**

Make sure if **NR** and **BR** was derived independently!

Marking transitions going to the g.s.

gabs -M InpFile

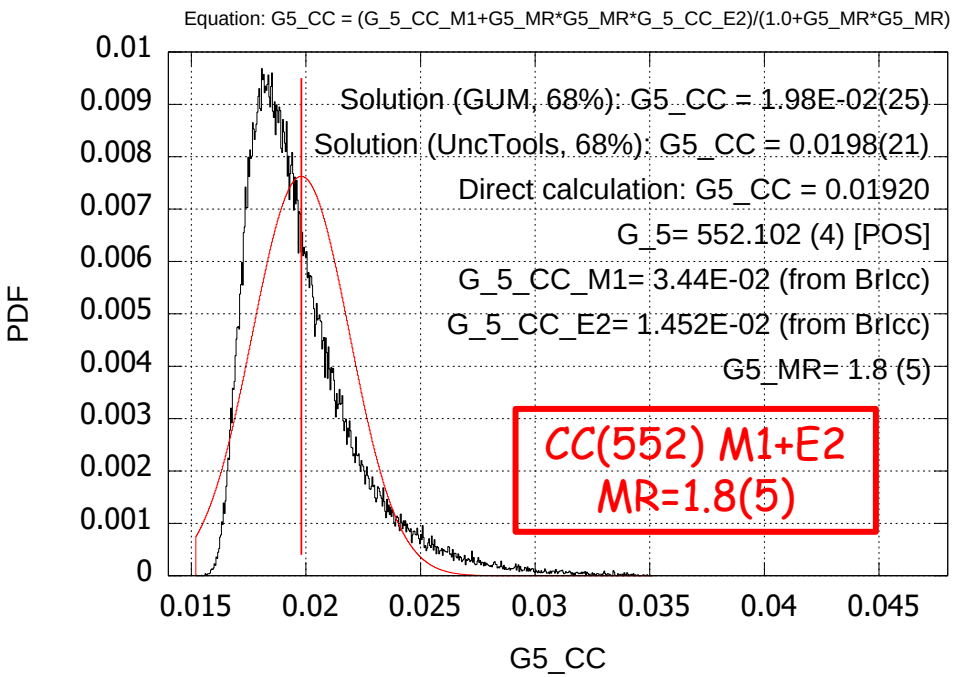
Command: gabs -m 80Br_B-EC.ens

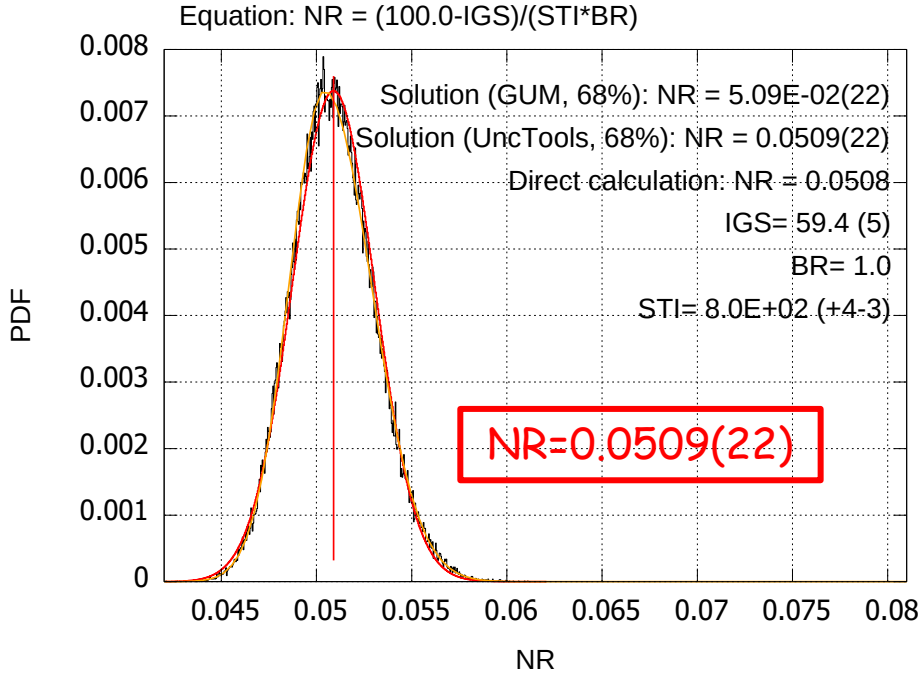
```
==========  GABS Version 12 [04-Apr-2019]  ==========
Report file:        80Br_B-EC.rpt
Loading input file: 80Br_B-EC.ens
  Data set: 80BR B- DECAY (17.68 M)
  Data set: 80BR EC DECAY (17.68 M)
Searching for ground state transitions * * * * *
ENSDF input file: 80Br_B-EC.ens
New ENSDF   file: 80Br_B-EC.in
Report file:      80Br_B-EC.rpt
NR & BR fields on the Normalisation record will be blanked

Data set: 80BR B- DECAY (17.68 M)
   Transitions to the G.S.
   Level         GE         RI       DRI   TI         DTI   Flag
   616.6         616.3      100              100.2            Y     <W> TI calculated from RI & CC
   1256.0        1256.2     1.1      1     1.10       10    X     <W> No CC given, TI = RI !

Data set: 80BR EC DECAY (17.68 M)
   Transitions to the G.S.
   Level         GE         RI       DRI   TI         DTI   Flag
   665.8         665.8      16.1     13    16.1       13    X     <W> No CC given, TI = RI !

   Summed intensities       117.2    13    117.4      13

Calculations completed
```

Benchmarking GABS

^{177}Lu B-
12 G`s for
normalisation

	GABS	Python	UncTools
Input file	gabs-test.ens	pycalc-test.py	gabs-test.unc
NR	0.0508(21)	0.0508(21)	0.0509(22)
%IG(150.399)	18.0 (5)	18.0 (5)	18.0 (5)





Caution: For low energy transitions **CC** can be large and **DTI** could be asymmetric

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GABS v12

- GABS program logic simplified
- Code re-written in F90
- Input data error handling improved
- New operation modes: -F, -C, -M
- Calculations for single data set fully tested
- Calculations for multiple data sets is under development
- GABS manual need to be updated

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DBR & DNR for data-set 2/3

$$BR = \frac{\frac{100}{100-IGS1} * TI1}{\frac{100}{100-IGS1} * TI1 + \frac{100}{100-IGS2} * TI2 + \frac{100}{100-IGS3} * TI3};$$

σ_{br} =

```
((D[BR, IGS1] * ΔIGS1) ^ 2 + (D[BR, IGS2] * ΔIGS2) ^ 2 + (D[BR, IGS3] * ΔIGS3) ^ 2 + (D[BR, TI1] * ΔTI1) ^ 2 +
   (D[BR, TI2] * ΔTI2) ^ 2 + (D[BR, TI3] * ΔTI3) ^ 2 ) ^ 0.5;
FullSimplify[σbr]
```

$$\Big(\big((-100+IGS1)^4 (-100+IGS2)^2 (-100+IGS3)^2 ((-100+IGS3)\,TI2 + (-100+IGS2)\,TI3)^2 \Delta TI1^2 + (-100+IGS1)^2 TI1^2 \big(2 (-100+IGS2)^3 (-100+IGS3)^3 TI2\,TI3\,\Delta IGS1^2 + (-100+IGS3)^4 TI2^2 \big((-100+IGS2)^2 \Delta IGS1^2 + (-100+IGS1)^2 \Delta IGS2^2\big) + (-100+IGS2)^2 \big((-100+IGS2)^2 TI3^2 \big((-100+IGS3)^2 \Delta IGS1^2 + (-100+IGS1)^2 \Delta IGS3^2\big) + (-100+IGS1)^2 (-100+IGS3)^2 \big((-100+IGS3)^2 \Delta TI2^2 + (-100+IGS2)^2 \Delta TI3^2\big)\big)\big)\big) \Big/ \Big((-100+IGS1)^2 ((-100+IGS2)(-100+IGS3)\,TI1 + (-100+IGS1)((-100+IGS3)\,TI2 + (-100+IGS2)\,TI3))^4\Big)\Big)^{0.5}$$

$$NR = \frac{100}{\left(\frac{100}{100-IGS1} * TI1 + \frac{100}{100-IGS2} * TI2 + \frac{100}{100-IGS3} * TI3\right) * \frac{100}{100-IGS1} * (TI1)};$$

σ_{nr} =

```
((D[NR, IGS1] * ΔIGS1) ^ 2 + (D[NR, IGS2] * ΔIGS2) ^ 2 + (D[NR, IGS3] * ΔIGS3) ^ 2 + (D[NR, TI1] * ΔTI1) ^ 2 +
   (D[NR, TI2] * ΔTI2) ^ 2 + (D[NR, TI3] * ΔTI3) ^ 2 ) ^ 0.5;
FullSimplify[σnr]
```

$$0.01\Big(\big((-100+IGS1)^2 (-100+IGS2)^2 (-100+IGS3)^2 TI1^2 (2 (-100+IGS2)(-100+IGS3)\,TI1 + (-100+IGS1)((-100+IGS3)\,TI2 + (-100+IGS2)\,TI3))^2 \Delta IGS1^2 + (-100+IGS1)^6 (-100+IGS3)^4 TI1^2 TI2^2 \Delta IGS2^2 + (-100+IGS1)^6 (-100+IGS2)^4 TI1^2 TI3^2 \Delta IGS3^2 + (-100+IGS1)^4 (-100+IGS2)^2 (-100+IGS3)^2 (2 (-100+IGS2)(-100+IGS3)\,TI1 + (-100+IGS1)((-100+IGS3)\,TI2 + (-100+IGS2)\,TI3))^2 \Delta TI1^2 + (-100+IGS1)^6 (-100+IGS2)^2 (-100+IGS3)^4 TI1^2 \Delta TI2^2 + (-100+IGS1)^6 (-100+IGS2)^4 (-100+IGS3)^2 TI1^2 \Delta TI3^2\big) \Big/ \Big(TI1^4 ((-100+IGS2)(-100+IGS3)\,TI1 + (-100+IGS1)((-100+IGS3)\,TI2 + (-100+IGS2)\,TI3))^4\Big)\Big)^{0.5}$$