

Deconvolution of Gamma-Ray Peak Doublets as a Function of Peak Separation and Relative Amplitude

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Abstract

When gamma-ray lines overlap, it is necessary to use deconvolution techniques to determine the best peak areas for the individual components. The ability of the least square fitting technique to determine the peak area is shown. The spectra used contained manufactured doublets of separation from less than the FWHM to more than FWHM and relative amplitudes of 1:1 and 1:1000. The small peak area is studied on both the low and high energy side of the large peak areas.

Spectra

In the development of software to analyze gamma-ray spectra and methods for testing the efficacy of this software the deconvolution of doublets or higher multiplets has always been an important (if not necessary) consideration. The deconvolution test has also been included in international standards for gauging the performance of the analysis software. One interesting recent requirement was the separation of $\text{Ag}^{110\text{m}}$ from Cs^{137} .

The doublet spectra were manufactured by summing (channel by

channel) two separate singlet spectra where one of the singlet centroid channel was moved by using a biased amplifier. The singlet spectra were collected on an EG&G ORTEC GMX 18195 detector. This detector is an n-type with thin entrance window to allow collection of low energy photons. Nuclides were chosen with isolated single gamma rays over as wide an energy range as possible. The lowest energy isolated gamma ray was the 123 keV line from Eu^{154} ; the highest energy was 1274 keV from Na^{22} .

Each nuclide was collected separately. The different area peaks were collected by changing the collection live time. The different position peaks were collected by measuring the FWHM of the large area peak and adjusting a bias amplifier to shift the centroid by approximately 1/2, 1, and 2 times the FWHM. Each peak was collected separately, resulting in 20 spectra for each energy of interest. Figure 1 shows a set of typical peak areas.

The data were all collected with the same gain of approximately 0.25 keV per channel. This is a commonly used energy scale and results in 2 MeV full scale for 8K channels. The combined system noise adds to the detector resolution of 1.95 keV (at 1332 keV) giving a total resolution of 1.4 keV at 123 keV and 2.18 keV at 1275 keV. This corresponds to between 5 and 6 channels in the FWHM at 123 keV and to between 8 and 9 channels at 1275 keV. This is about the lower limit for the number of channels per peak for a reasonable fit of the data to a Gaussian shape.

The collection times were selected so that the total area in the shortest collection time for the weakest source was a reasonable number. The set of collection times (one time for each of the different peak areas) was the same for all the sources, so for the stronger sources, each of the individual peak areas were larger than the corresponding weak-source peak areas for a given counting time. This gave a range of peak areas for the deconvolution of from 37 counts to 300000 counts. These peak areas and the summed spectra are more representative of typical laboratory spectra than computer-generated peak areas and spectra because the peak shapes are the detector peak shapes and the peak counts and the background counts have the necessary statistical variation.

The reference areas for the singlet components were obtained by analyzing the individual spectra using the same parameters for energy and shape calibration as would be used for the deconvolution. The counting uncertainty in the smaller peak areas causes the shape of the peak to vary from the predicted shape for some of these peaks and this poor shape (of the smaller component) contributes to the poor fit of resultant multiplets. Figure 2 shows a set of singlet spectra with the fitted peak. The actual peak shape is close to the Gaussian shape in most cases.

A set of the summed doublet spectra and the fits are shown in Figures 3 and 4.

Deconvolution Method

The deconvolution proceeds along these steps: 1) background determination, 2) construction of unit-height peak shapes, and 3) least square fit of the unit peak shapes to the spectrum.

The first approximation to the background is constructed by drawing a straight line between the average background below the multiplet to the average background above the multiplet. The average background below the multiplet is the minimum value of the 5-point average in the range between the centroid of the lowest energy component of the multiplet and a point corresponding to 1.5 times the FWHM below the lowest energy component. The limit of 1.5 FWHM is taken to be below the peak contribution. The average background above the multiplet is the minimum value of the 5-point average in the range between the centroid of the highest energy component of the multiplet and a point corresponding to 1.5 times the FWHM above the highest energy component. The background values are assigned to the center channels of the 5 points. This background is then subtracted, channel-by-channel, from the original data.

A peak, with unit area, is calculated for each peak to be included in the least-squares fit. The centroid energy of each peak is given in a table. A Gaussian peak shape is used, so the only shape parameter is the FWHM which is determined in a separate calibration process by fitting well-formed calibration peaks over the energy range of interest. The FWHM is stored as a quadratic fit to the energy versus FWHM curve. The contribution of every peak in the table is calculated for all channels of the test spectrum included in the doublet region. The doublet region is all the channels bounded by the high and low background channels.

The net spectrum (of i -channels) can be represented as a linear sum of the Gaussian peaks with the weighting factors of each component proportional to the area of the component peak. The weighting factors are determined by the fitting of the unit-area peaks to the test spectrum.

The result, that is the area of the J -th component of the multiplet, is the J -th weighting factor in the sum times the unit-height area for the Gaussian centered at peak position J .

If the slope of the background across the peak-multiplet region is more negative than the slope of the background above the peak-multiplet region, a stepped background is added to the original background (in the peak-multiplet region) according to the

relative heights of the peaks. A new net spectrum is calculated and the region is refit.

Figures 5, 6 and 7 show the results of some deconvolutions.

Results

A total of 100 doublets over the range of peak width and separation were resolved. Figure 8 shows the average error in the calculated area versus the known area, expressed as percent of the known area. As can be seen in the figure, the error is quite small except in the limit of the amplitude ratio of 1:1000 and separation of less than FWHM.

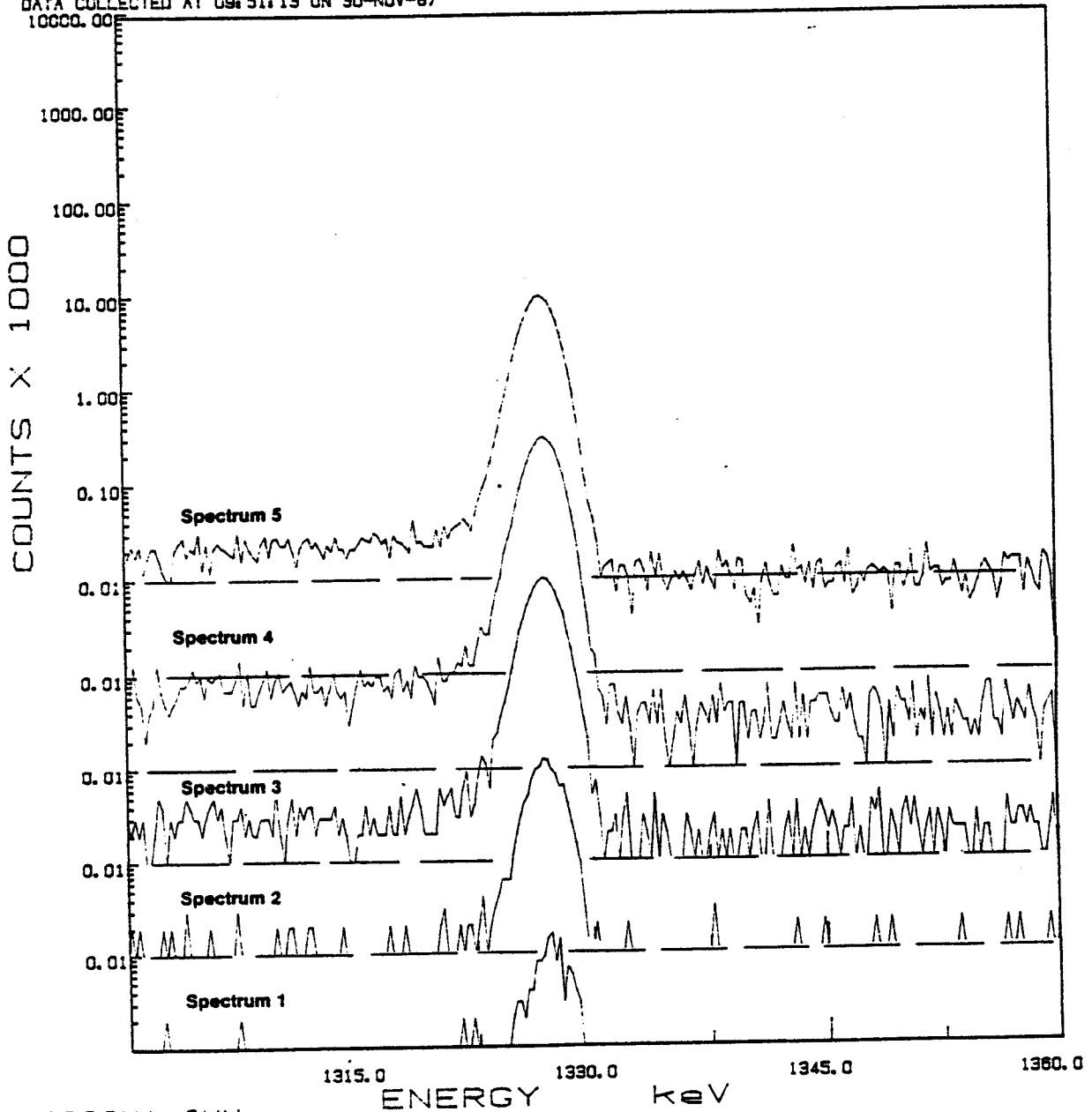
When the amplitude ratio is in the range of 1:1000 or 1:100, the error in the large peak is often greater than the total area of the small peak. Figure 9 shows the difference between the calculated area and known area expressed in units of the counting error in the multiplet area.

Figure 10 shows the same result expressed as a percentage of the total counts in the doublet.

As can be seen in Figures 8 through 10, the ability to separate two peaks can be reliably accomplished until the peak amplitude ratio approaches 1:1000 and the separation is less than the FWHM.

There is no distinct difference between the two cases where the small peak is above or below the larger peak. Further studies will concentrate on improving this limit by increasing the number of channels per peak.

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Fig. 1 A Typical Set of Spectra

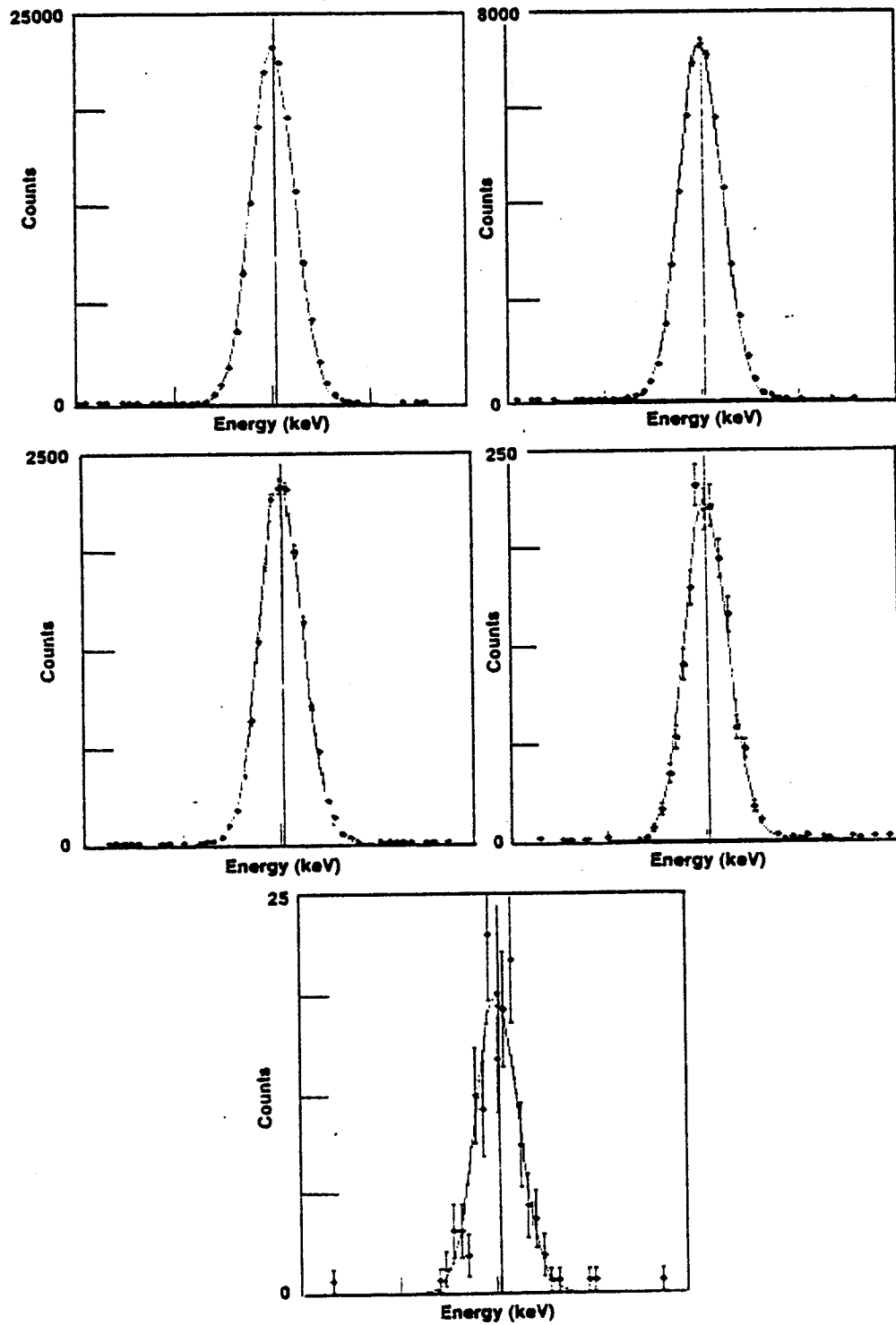


Fig. 2 Set of Fitted Singlets

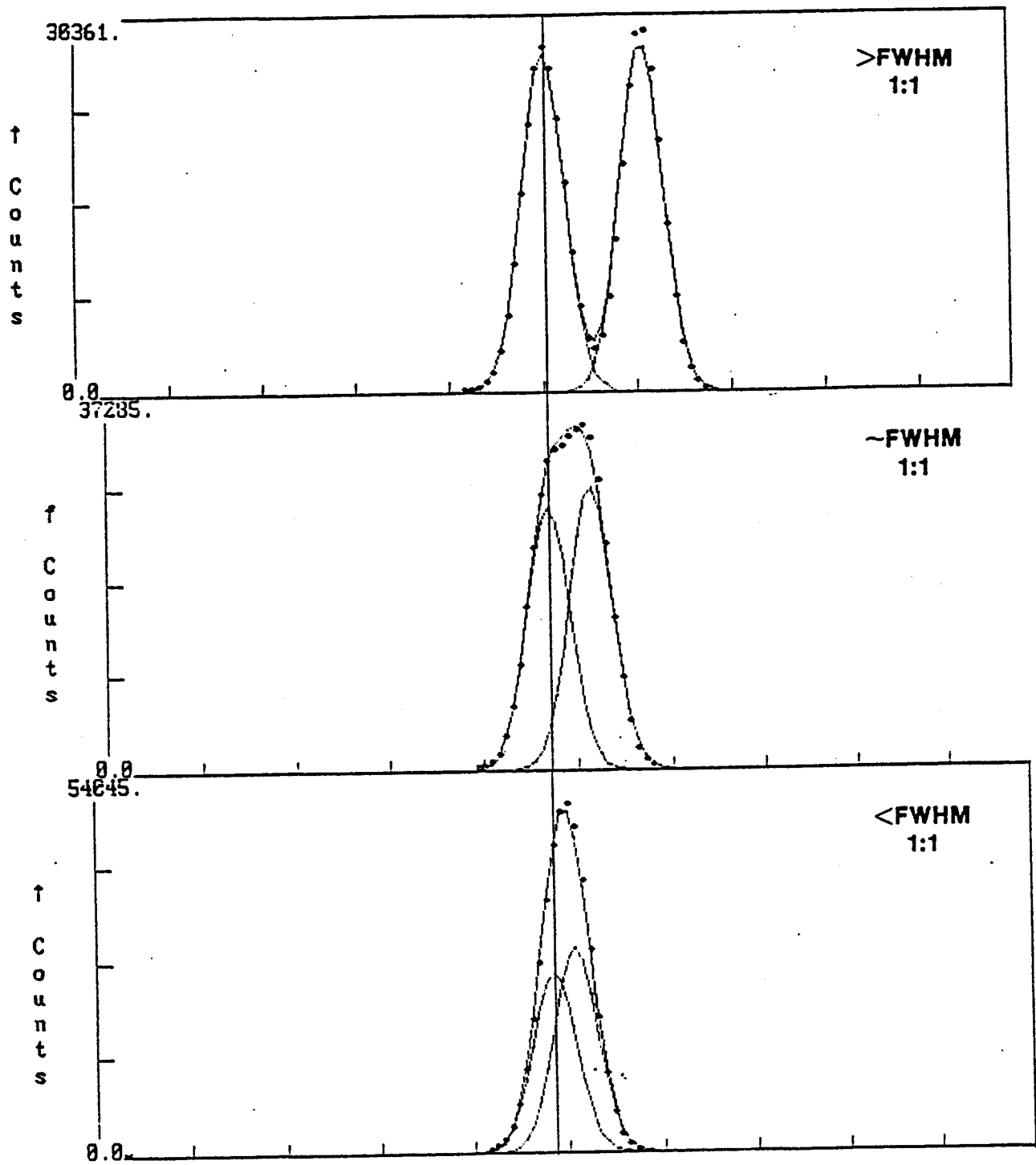


Fig. 3 Typical Doublet with Fitted Result

Note that the areas are the same, only the separation is changed.

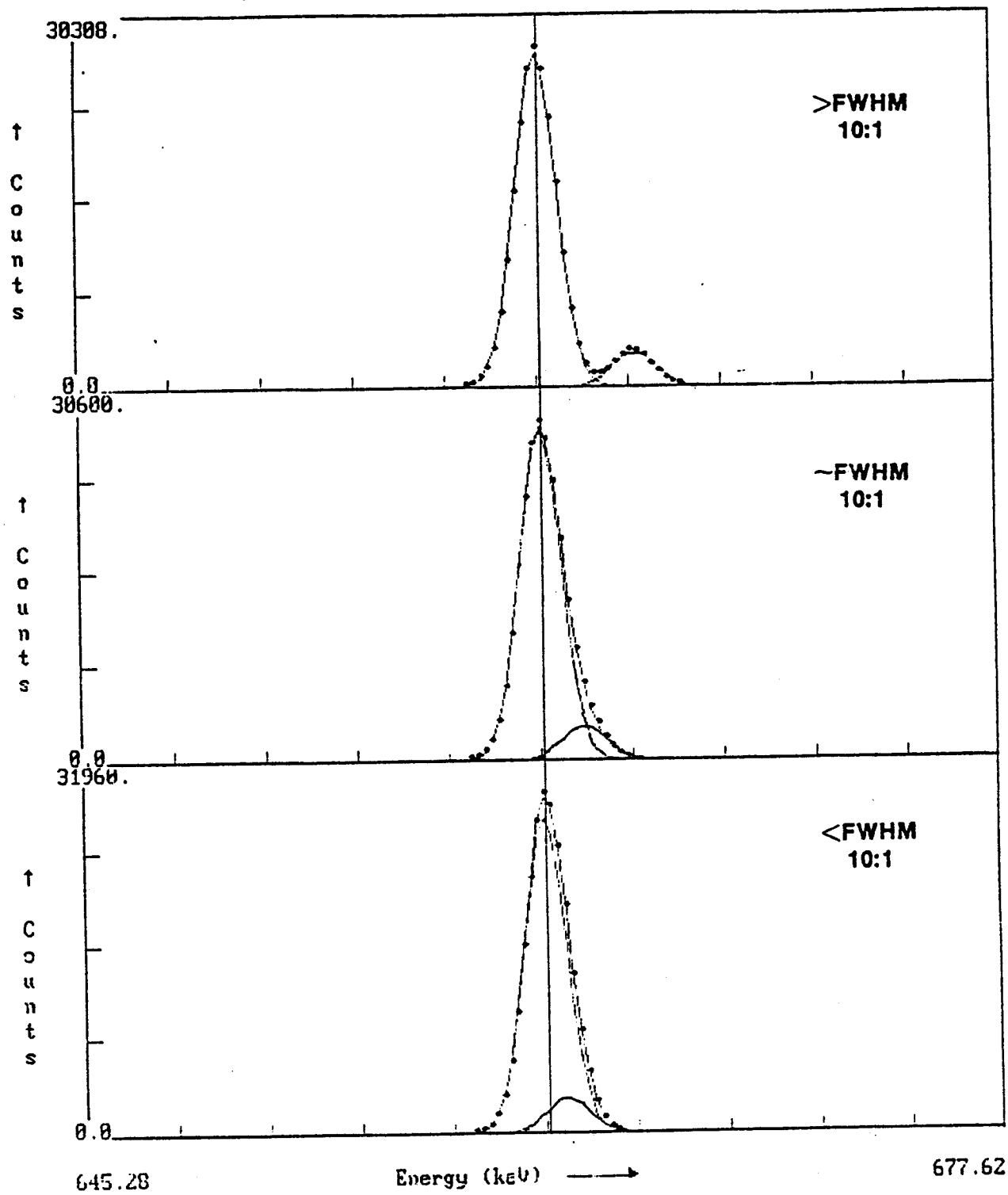


Fig. 4 Typical Doublet with Fitted Result

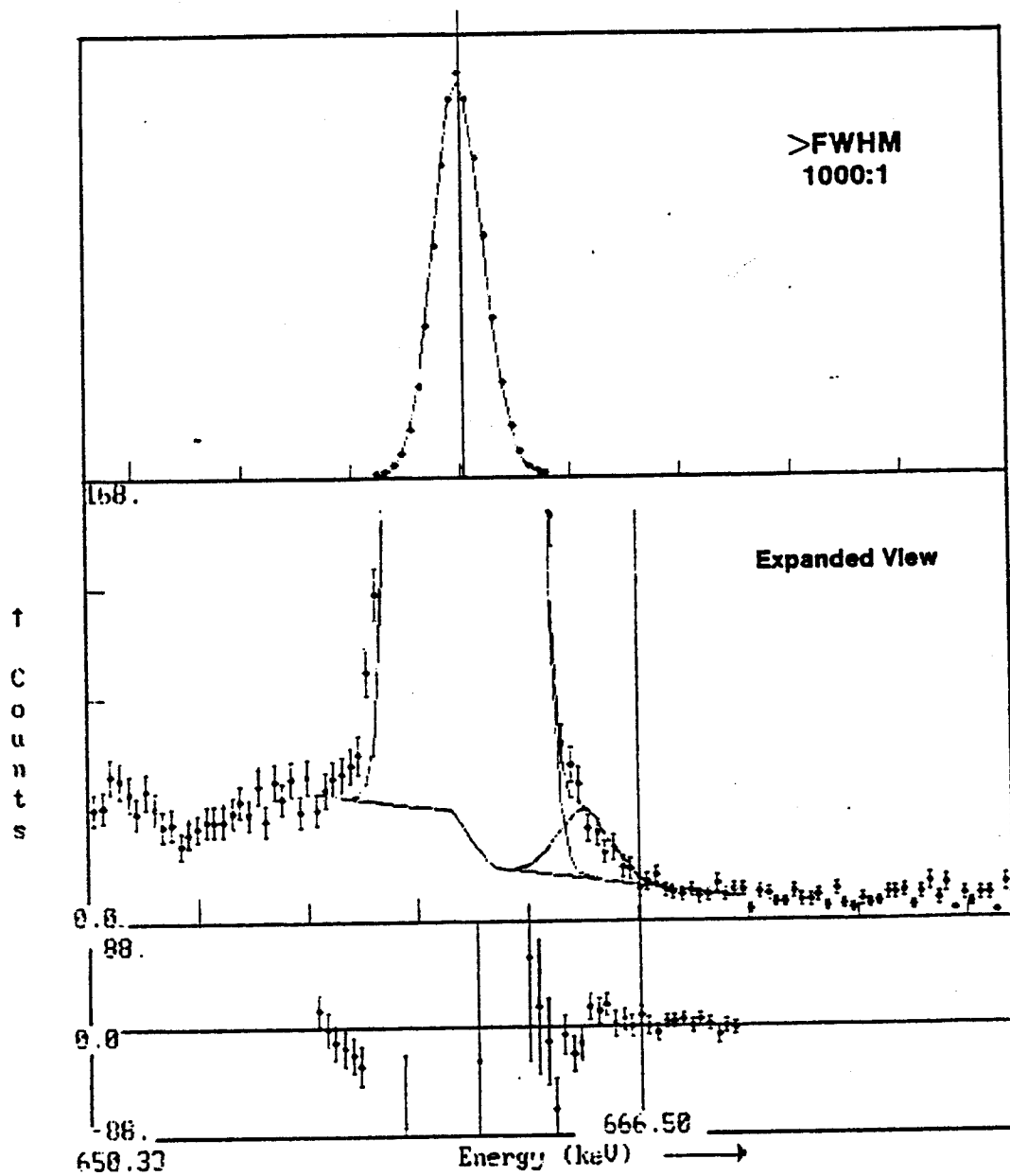


Fig. 5 Deconvolution Result for the Case of 1:1 and <FWHM

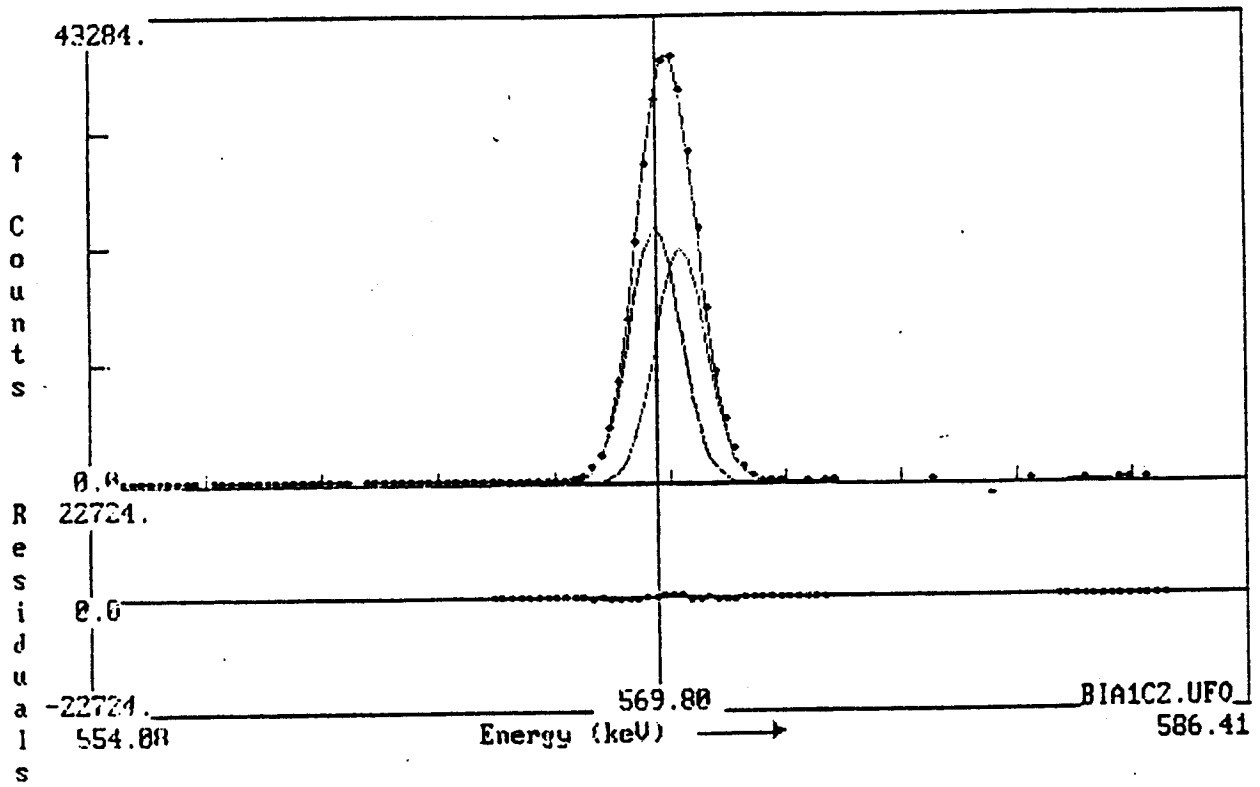


Fig. 6 Deconvolution Result for the Case of 1:1 and = FWHM

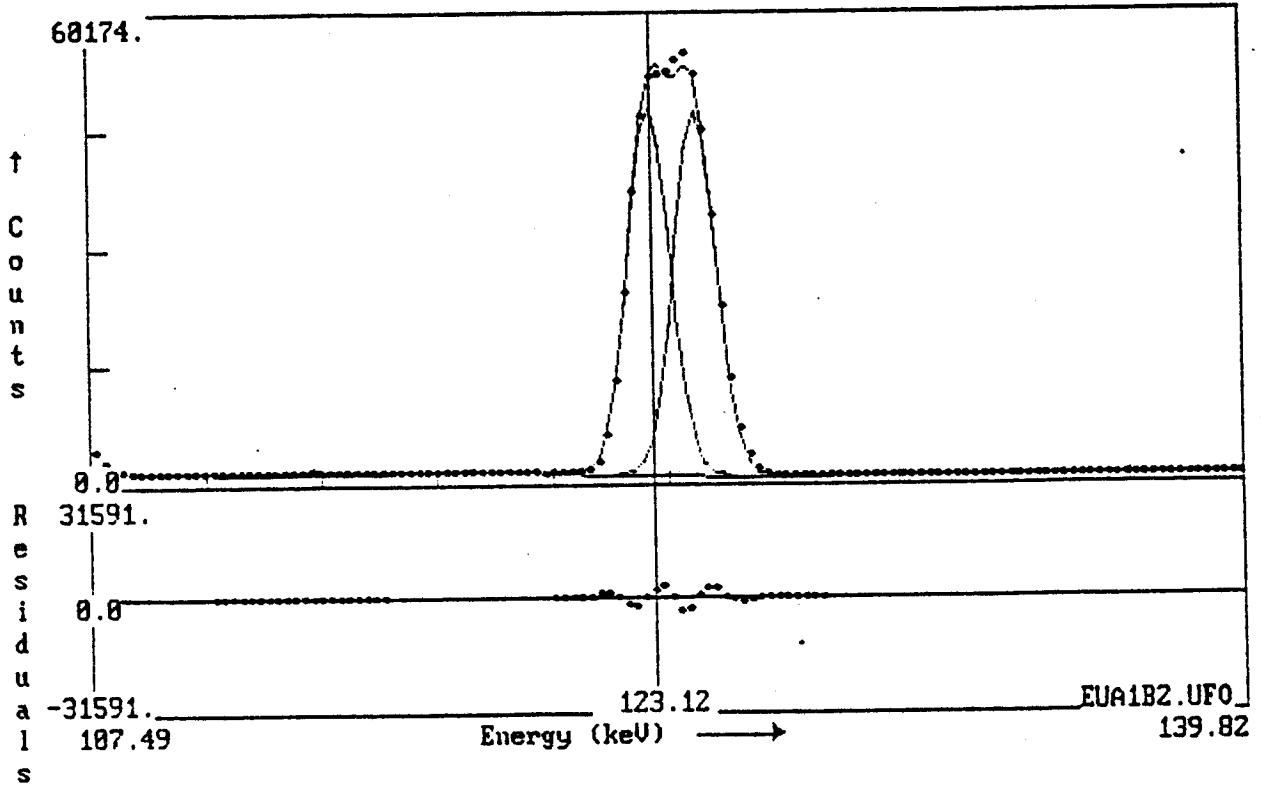


Fig. 7 Deconvolution Result for the Case of 1:1 and > FWHM

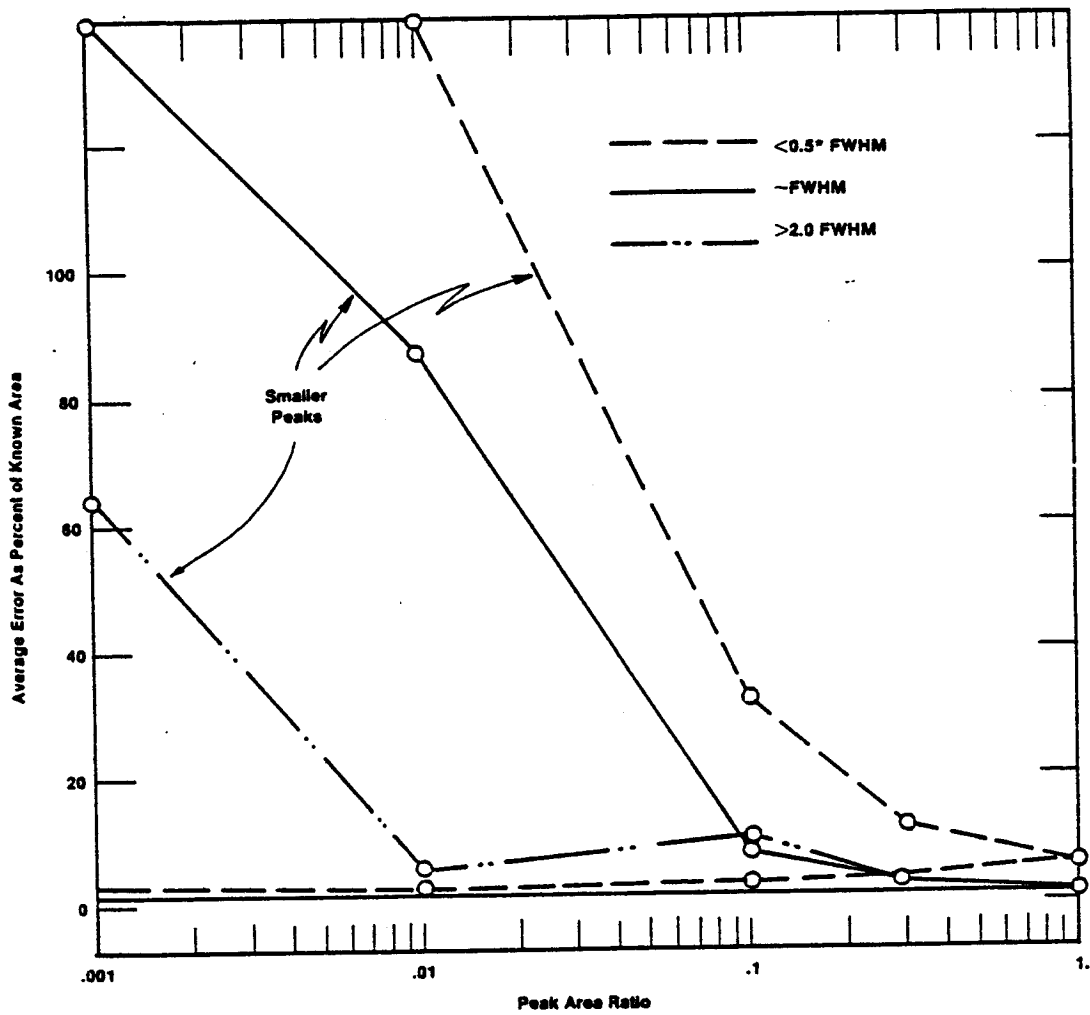


Fig. 8 Average Error in Calculated Area vs Given Area as Percent of Peak Area

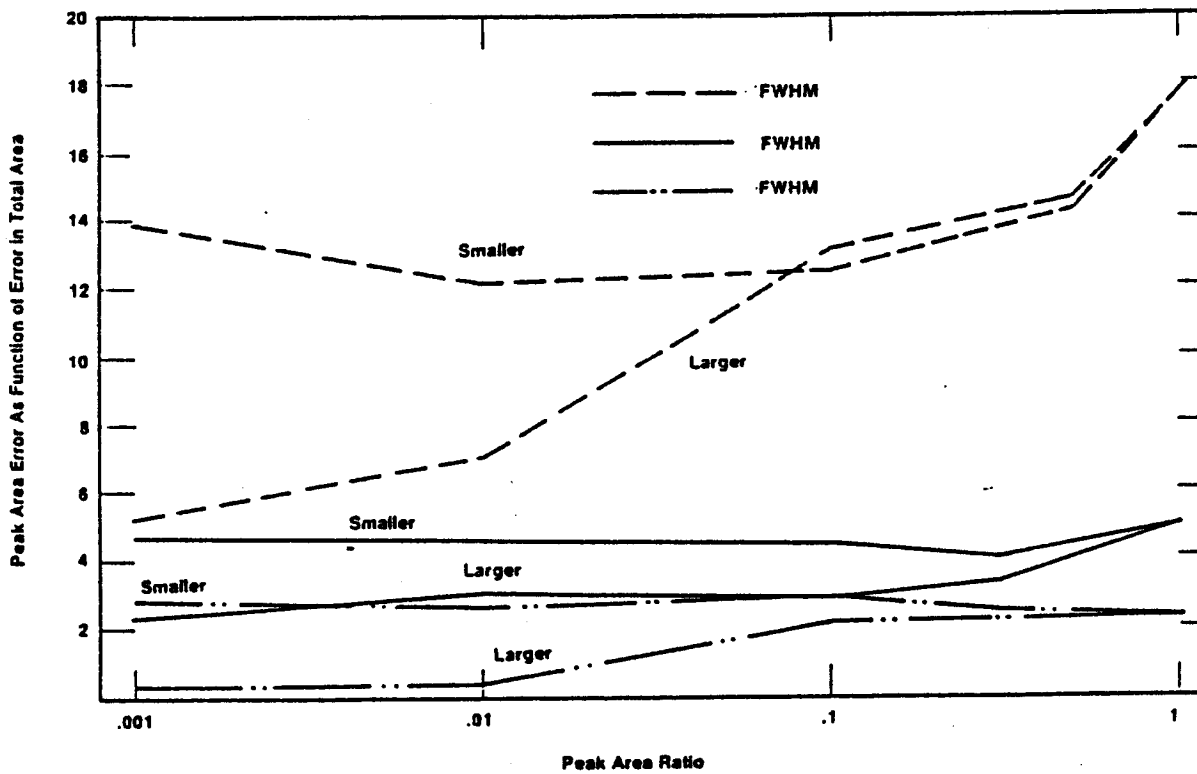


Fig. 9 Difference Between the Calculated Area and Known Area in Units of Counting Error in Multiplet area

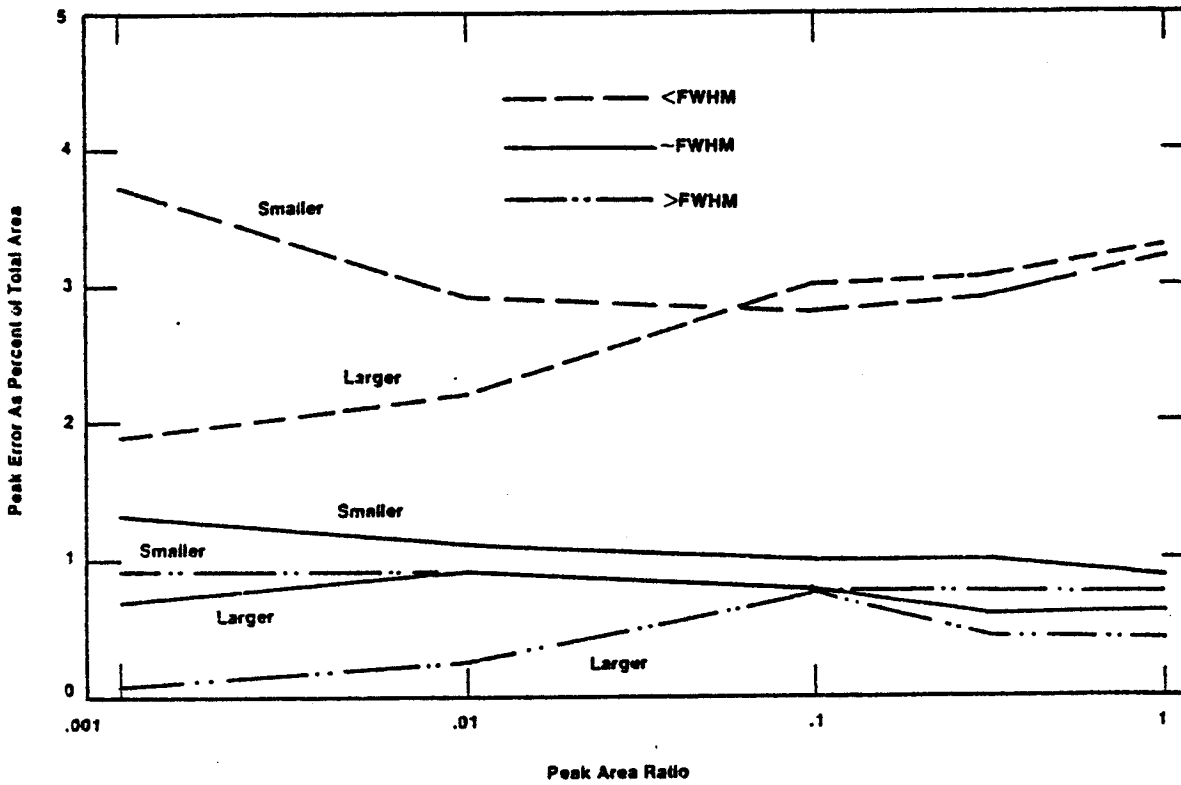


Fig. 10 Difference Between the Calculated Area and Known Area as Percent of Total Counts in Multiplet area