Synthetic Components

The display of the synthetic components can be controlled using the **Comp Index** field now available on the Components property page of the Quantification Parameter dialog window (Figure 1). The component index presents an additional numerical identifier associated with a component. When a component is created, the default value for the Comp Index field is -1, however the integer value entered for a component is used to collect together components with some commonality, such as both components belonging to the a doublet pair or all components corresponding to chemically shifted peaks for a given electronic configuration (e.g. C 1s).

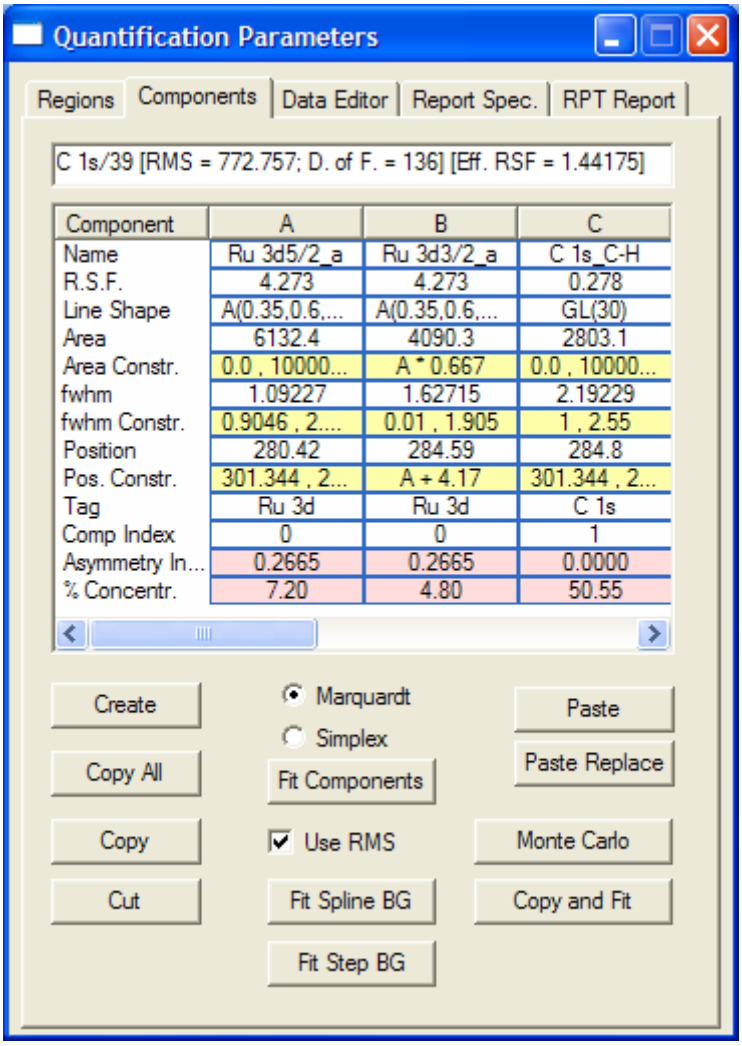

Figure 1

While the primary function of the Comp Index field is to plot components with the same colour, the Comp Index should be viewed as an association which may be exploited in other contexts. For example, if the FWHM constraint is specified as *link*, then all

components with the same Comp Index will have their FWHM constraint adjusted to ensure all components with the same Comp Index have the same FWHM as the component for which the key word *link* was entered.

Components are plotted using the Custom palette of colours viewed using the Colour dialog window available from the Colour property page of the Tile Display Parameters dialog window. The Custom palette consists of sixteen colours, each of which are user definable, and are referenced via the Comp Index field using the indices 0 to 15. When the use of the Comp Index is enabled, the default value for the Comp Index, namely -1, causes the components to be plotted using the colour with index 15. All other indices between 0 and 15 will select the colours from the Custom Palette from left to right and then top to bottom, as seen on the Colour dialog window (Figure 2).

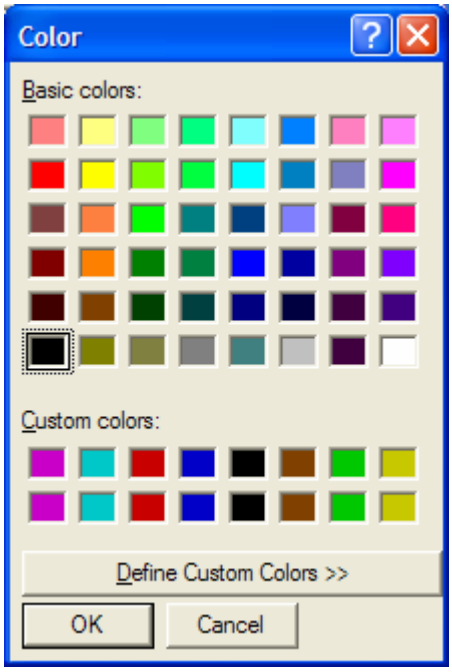

Figure 2

The set of components displayed in Figure 3 correspond to the Custom palette in Figure 2. While each component is identifiable using the annotation component table colour coded for each of the components using the custom colours, it is sometimes more convenient to group together peaks to simplify the plot. For the data in Figure 3, the data envelope is attributed to four C 1s peaks and two chemically shifted doublet pair from the Ru 3d transition. Grouping peaks according to the nature of the transitions simplifies the display as seen in Figure 4.

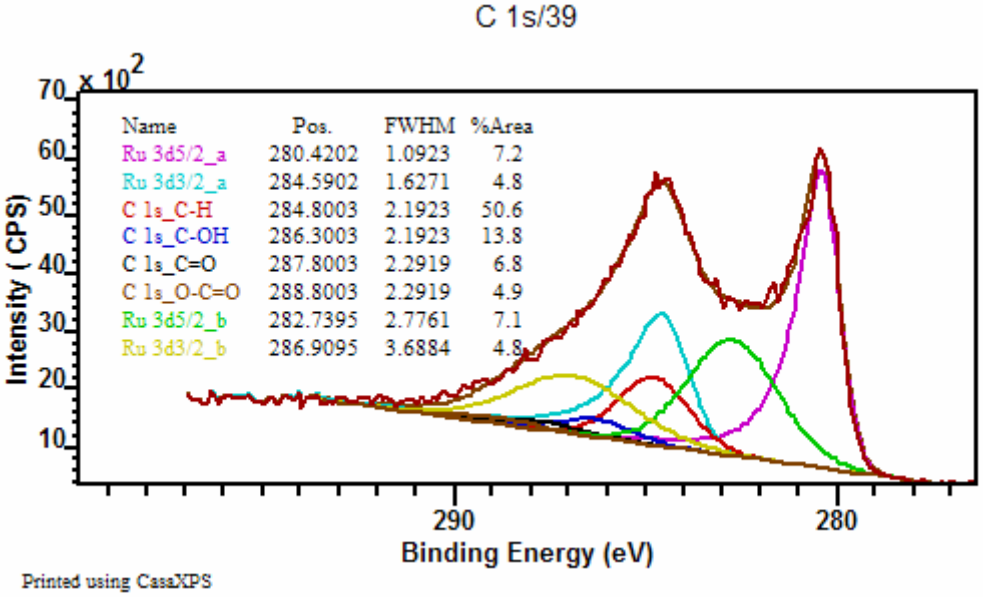

Figure 3

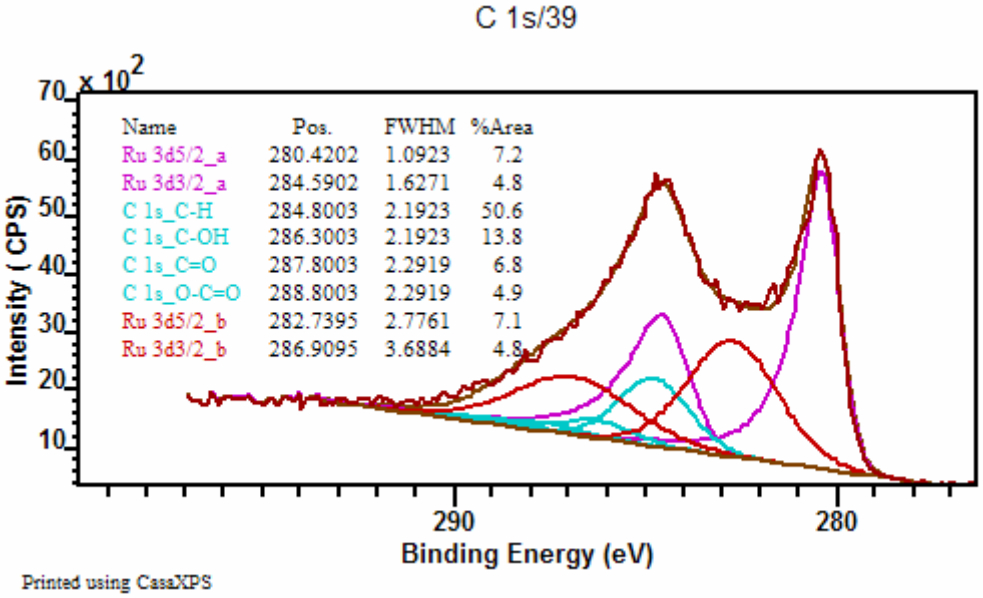

Figure 4

The mechanism for grouping component colours via the Comp Index is enabled using the tick boxes on the Colour property page of the Tile Display Parameter dialog window. Figure 5 shows the appropriate tick box in the state suitable for the display in Figure 4. The components in Figure 4 are arranged so that the doublet pair Ru 3d 5/2_a and Ru 3d 3/2_a both have an index of 0, while the four C 1s components are assigned an index of 1 and the final pair of Ru 3d transitions Ru 3d 5/2_b and Ru 3d 3/2_b have an index of 2.

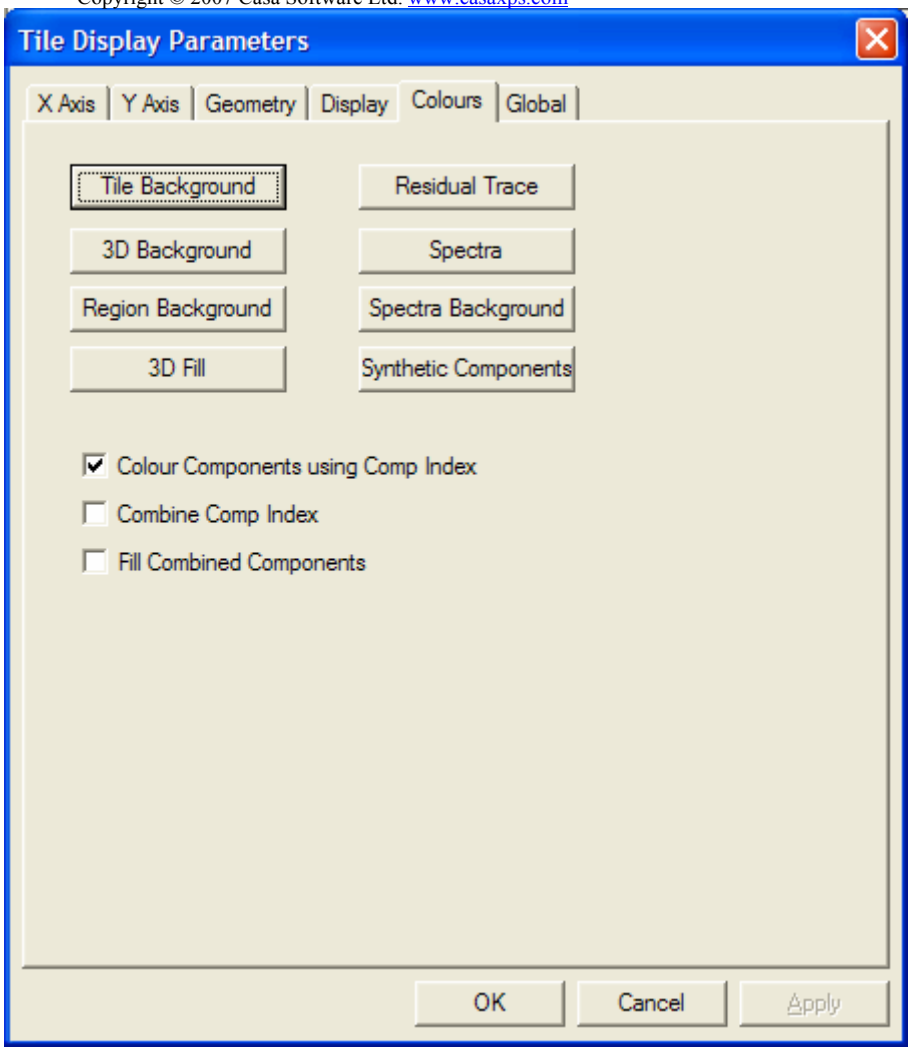

Figure 5

The reduction in colours used to illustrate the peak model simplify the display in Figure 4 compared to Figure 3; nevertheless a further simplification can be achieved by combining the intensities from peaks with the same Comp Index number. Rather than displaying the individual peaks, Figure 6 displays the intensity collected into curves for each of Comp Index values assigned to the components. For the data in Figure 6, each of the doublet pairs are assigned distinct indices; also, the set of C 1s peaks are differentiated from the Ru 3d peaks by a unique Comp Index value. As a result, three curves corresponding to the three different Comp Indices appear on the display. Collecting the components with common Comp Index values is achieved by ticking the Combine Comp Index tick box.

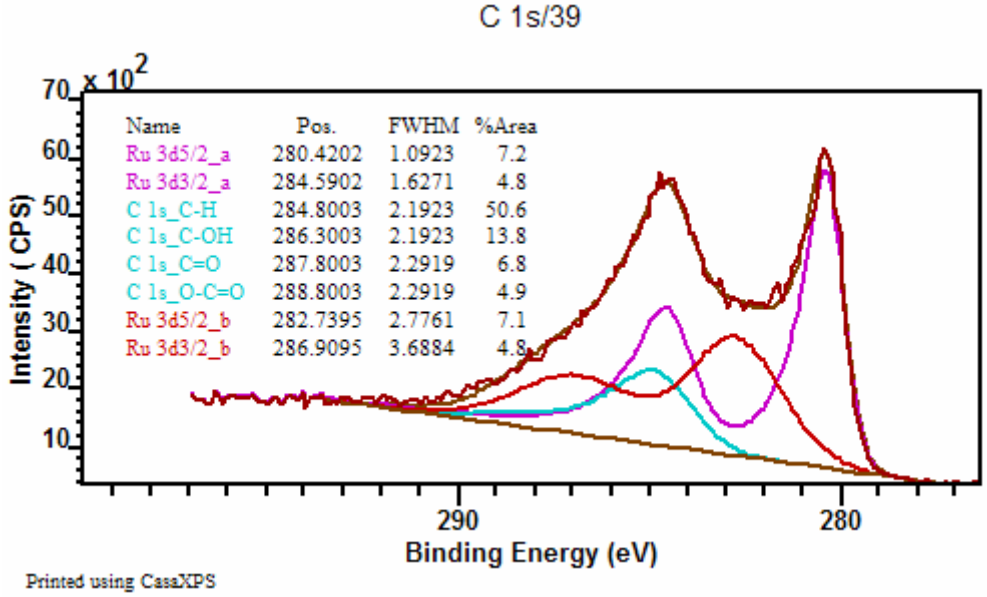

Figure 6

One further use of the Comp Index is to fill the components with the assigned colour as illustrated in Figure 7. The plot in Figure 7 uses distinct Comp Index values for each component to highlight the connection between the O 1s peak in the inset tile with the Si 2p oxide peak in the silicon data. The tick box Fill Combined Components is used to achieve the effect in Figure 7; the subtlety lies in the use of the Combine Comp Index tick box while using distinct Comp Indices to achieve the block fill of the individual components. The intended use of the Combine Comp Index is to provide an extension to the display of combined peaks such as those in Figure 6 using a block fill applied to the collective curve; however using the fill option with components each of which are assign unique Comp Indices provides a means of filling individual components.

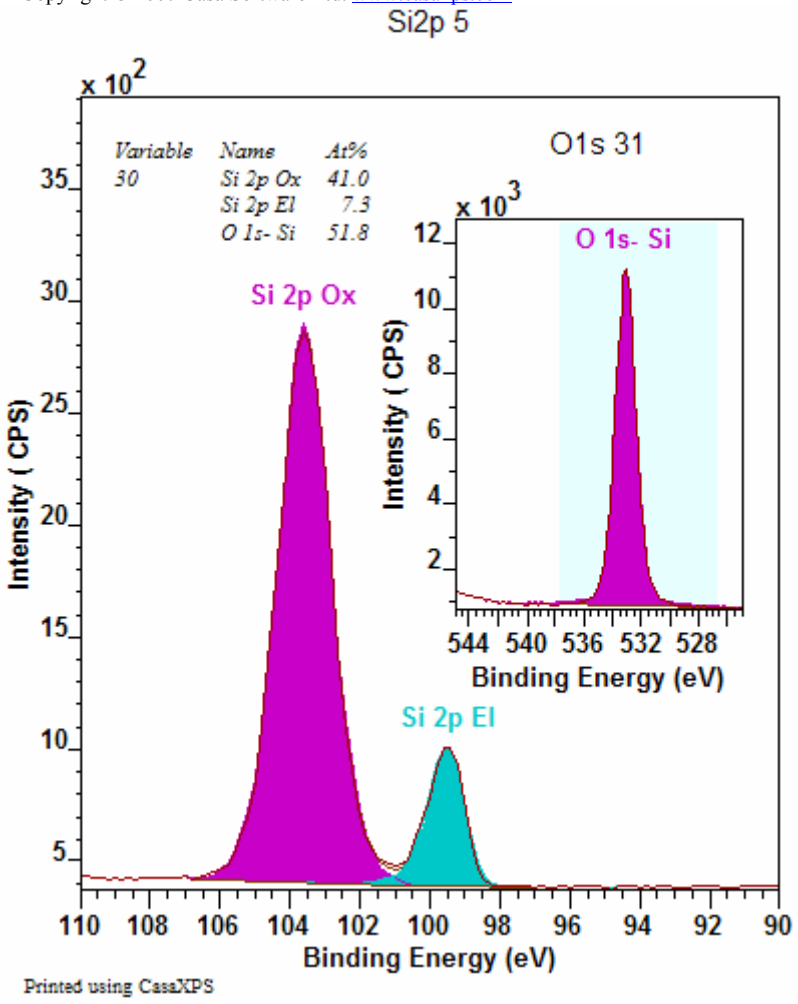

Figure 7