22. MINERALOGY ITERATIONS

Composition conversions, between substance (mineralogy) and elemental analyzes, are often needed in chemical R&D work. *The Mineralogy module easily converts mineralogical compositions into elemental ones, but is not always able to make reverse conversion*. Conversion can be made using the following procedure, see Fig. 1:

1. Type the species formulae into column A, use rows > 4. The species do not need to exist in the HSC database. However, you must use the HSC formula syntax.
2. Type the compositions in column D.
3. The elemental composition can be seen on row 4.

You can also give the total amount for the material in cell C4 as well as name in cell A1. Note that the user may edit only the cells with red fonts if **Format Red Font Shield** has been selected.

The conversion of the elemental composition of a substance into a mineralogical one is a more difficult task, for example due to small analytical errors. This module offers three tools for converting elemental analyzes into mineralogical ones.

1. Solve Method

The Solve method uses matrix-algebra to solve the mineralogy. It is useful if the given amounts of elements fit exactly to the given substances. The number of unknown compositions must also be the same as or less than the number of element balance columns.

An example of the Solve method is shown in Fig. 2 (file Example1.mnr). You can create this example from the previous one with the following procedure:

1. Press **Copy Row 4 to 3** button to copy elemental compositions from row 4 to 3.
2. **Type 1** to cells D5-D8, in order to wipe out the original compositions.
3. Press **Solve**. The results will be shown in column D. Usually the elements do not fit exactly to the given species, in these cases the Solve method may add some element rows to the system. These rows can be deleted by **Delete Row** selection.

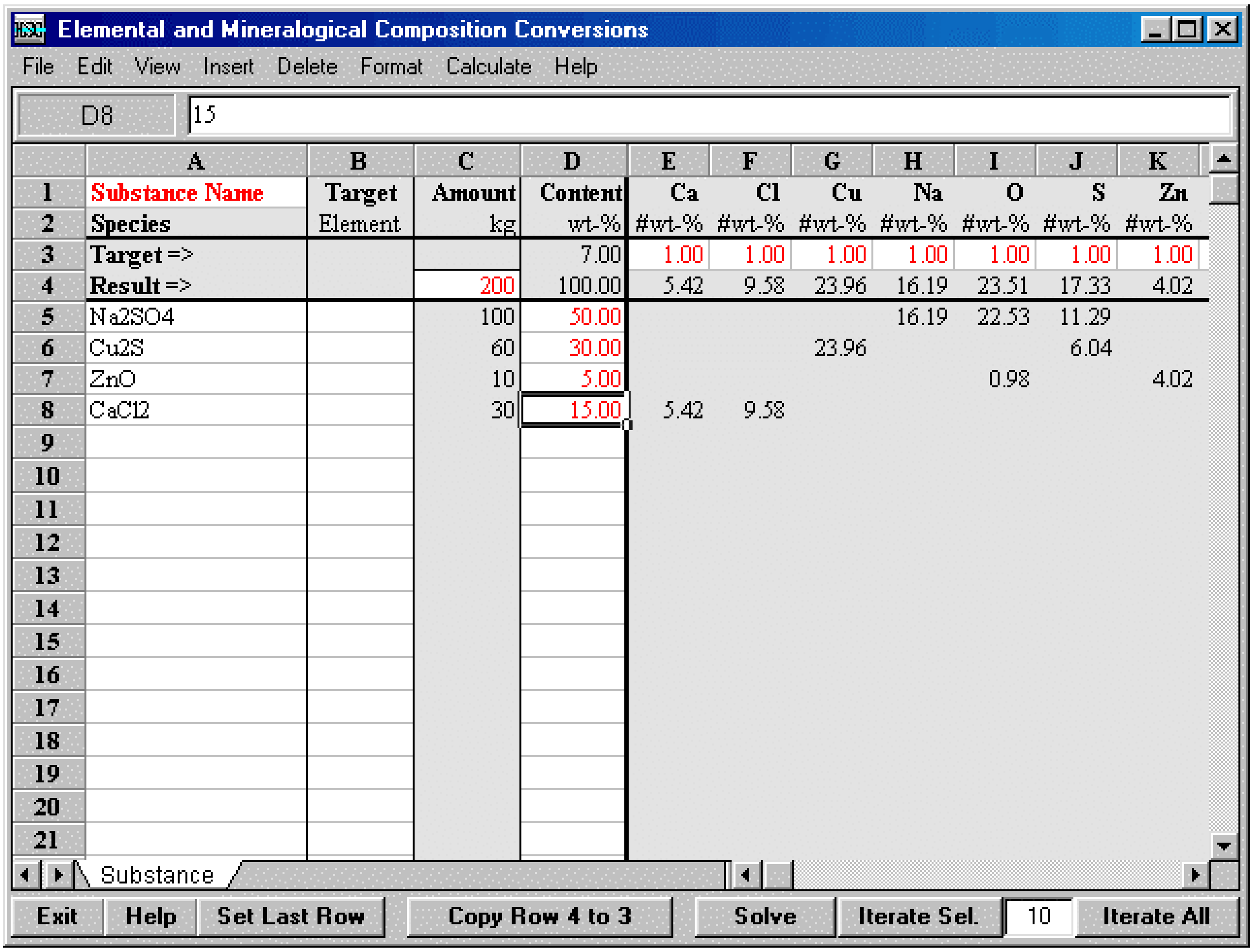
2. Automatic Iterative Method

The Automatic iterative method fits the given elements to the given substances by changing the species contents in order to reach the given element compositions. To carry out this conversion follow these steps, see Fig. 4:

1. Type species formulae to column A, use rows > 4.
2. Type elemental analyze to row 3, use columns > D.
3. Type the target elements, which will be used to iterate the species, into column B. Please do not use the same element for several species, otherwise manual iteration may be needed.
4. Press **Iterate All** to start iterations. Sometimes it is necessary to press this button several times in order to reach sufficient accuracy.

3. Manual Iterative Method

Sometimes the given elemental analysis does not fit with the given elements. In this case the user may search the approximate composition manually by changing the contents in column D, in order to reach a satisfactory match with the elemental analyzes in rows 3 and 4. **Iterate Sel** can be used to iterate individual rows.



	A	B	C	D	E	F	G	H	I	J	K
1	Substance Name	Target	Amount	Content	Ca	Cl	Cu	Na	O	S	Zn
2	Species	Element	kg	wt-%	#wt-%	#wt-%	#wt-%	#wt-%	#wt-%	#wt-%	#wt-%
3	Target =>			7.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
4	Result =>		200	100.00	5.42	9.58	23.96	16.19	23.51	17.33	4.02
5	Na2SO4		100	50.00				16.19	22.53	11.29	
6	Cu2S		60	30.00			23.96			6.04	
7	ZnO		10	5.00					0.98		4.02
8	CaCl2		30	15.00	5.42	9.58					
9											
10											
11											
12											
13											
14											
15											
16											
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19											
20											
21											

Fig. 1. Calculation of the elemental composition of a material mixture. The user has given the species names in column A and the contents in column D. The calculated result is shown on row 4.

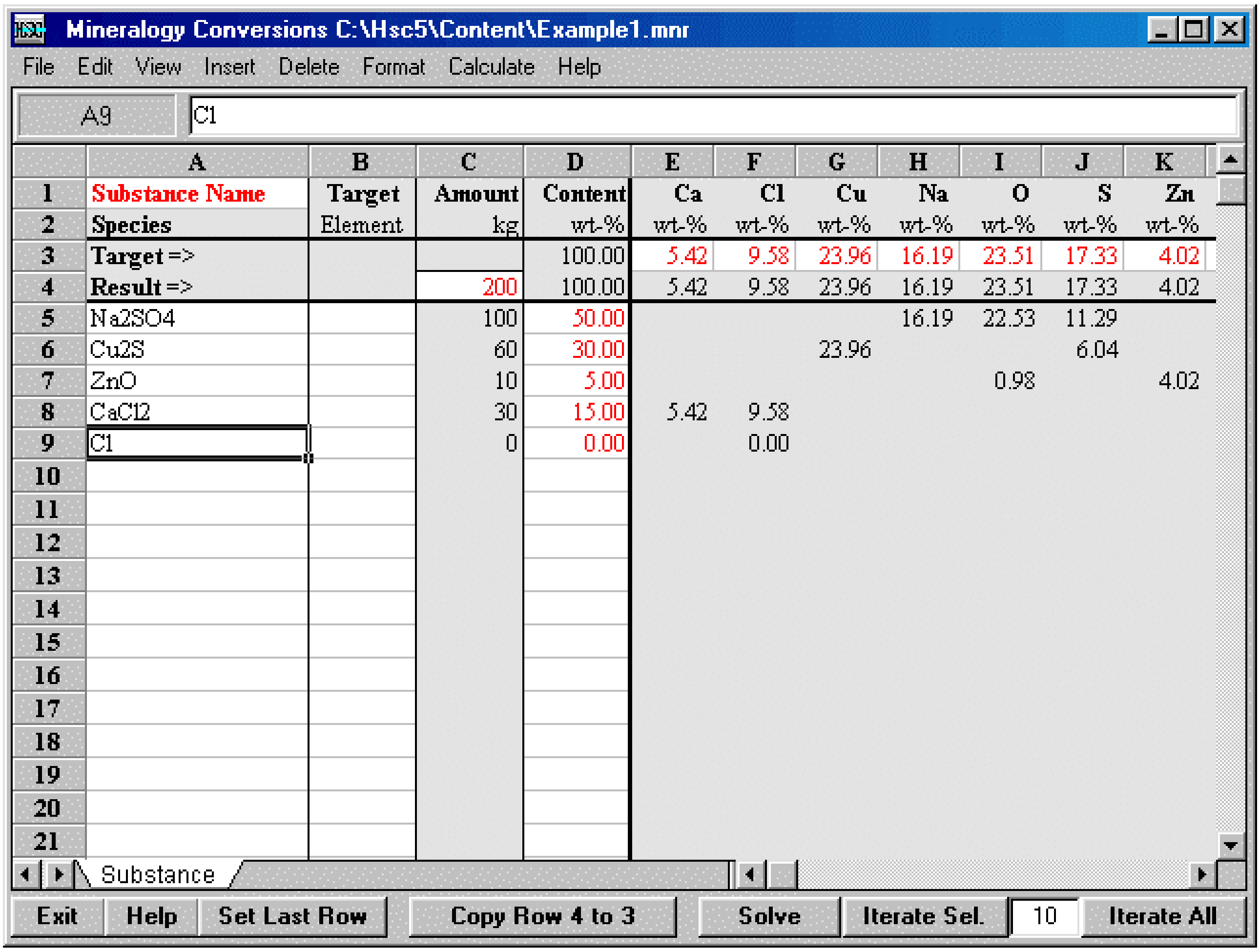


Fig. 2. Calculation of the species composition in column D using the elemental composition in row 3 by **Solve**.

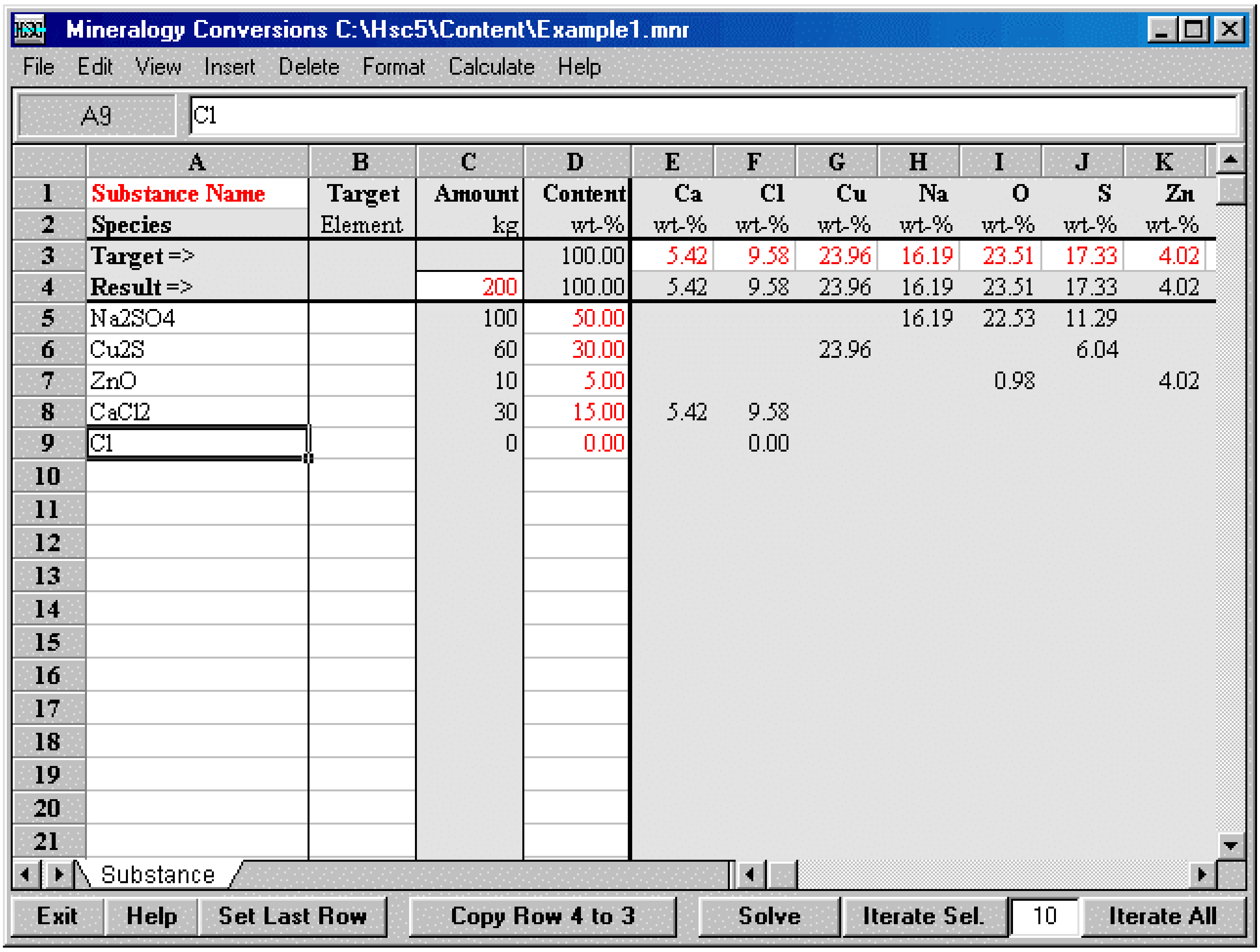
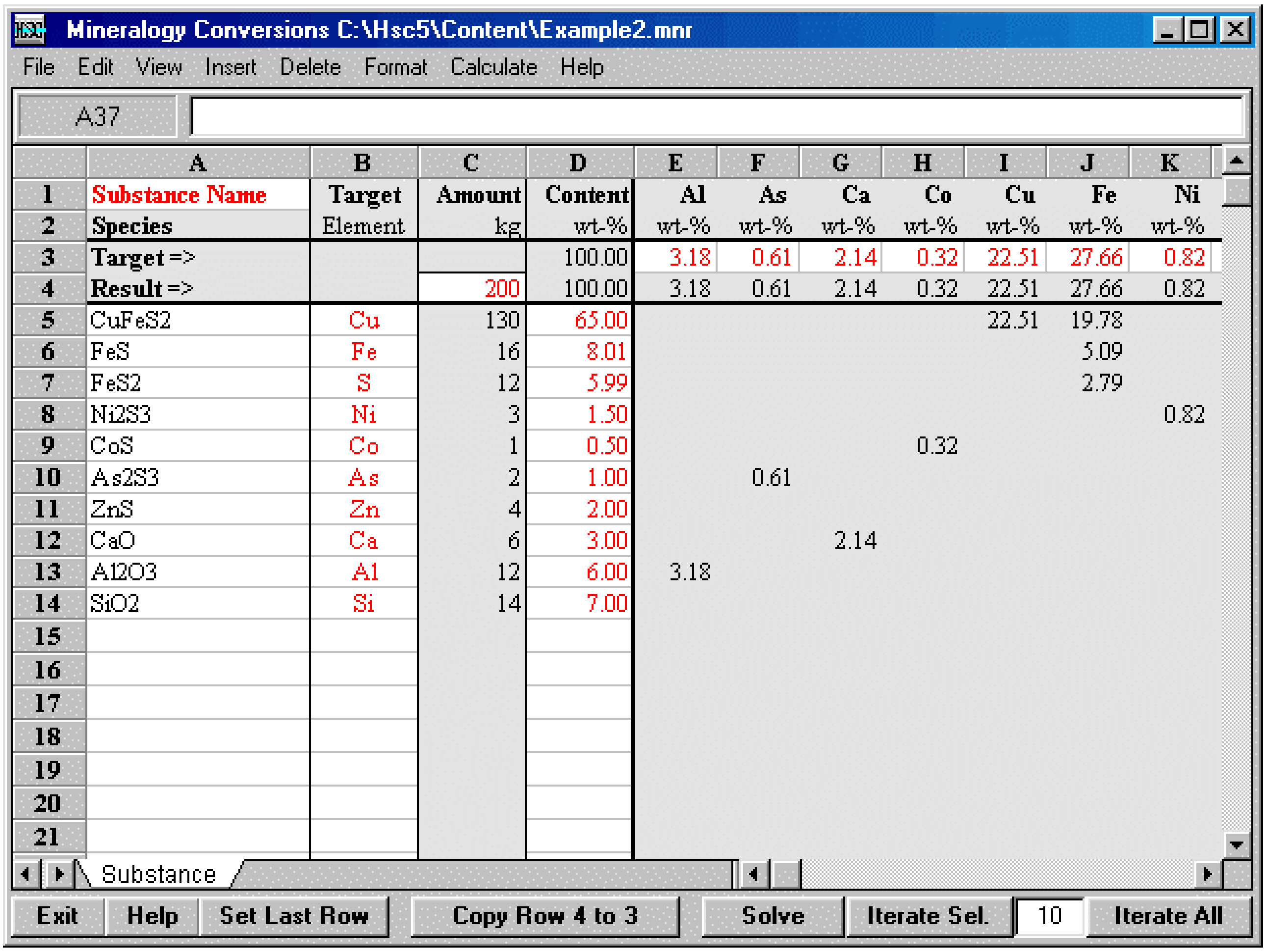


Fig. 3. Calculation of the elemental composition of a sulfide material. The user has given the species names in column A and the contents in column D. The result is on row 4.



	A	B	C	D	E	F	G	H	I	J	K
1	Substance Name	Target	Amount	Content	Al	As	Ca	Co	Cu	Fe	Ni
2	Species	Element	kg	wt-%	wt-%	wt-%	wt-%	wt-%	wt-%	wt-%	wt-%
3	Target =>			100.00	3.18	0.61	2.14	0.32	22.51	27.66	0.82
4	Result =>		200	100.00	3.18	0.61	2.14	0.32	22.51	27.66	0.82
5	CuFeS2	Cu	130	65.00					22.51	19.78	
6	FeS	Fe	16	8.01						5.09	
7	FeS2	S	12	5.99						2.79	
8	Ni2S3	Ni	3	1.50							0.82
9	CoS	Co	1	0.50				0.32			
10	As2S3	As	2	1.00		0.61					
11	ZnS	Zn	4	2.00							
12	CaO	Ca	6	3.00			2.14				
13	Al2O3	Al	12	6.00	3.18						
14	SiO2	Si	14	7.00							
15											
16											
17											
18											
19											
20											
21											

Fig. 4. Iteration of species compositions in column D on the basis of the elemental compositions in row 3 with **Iterate All**. The target elements in column B must be specified by the user.

Set Last Row

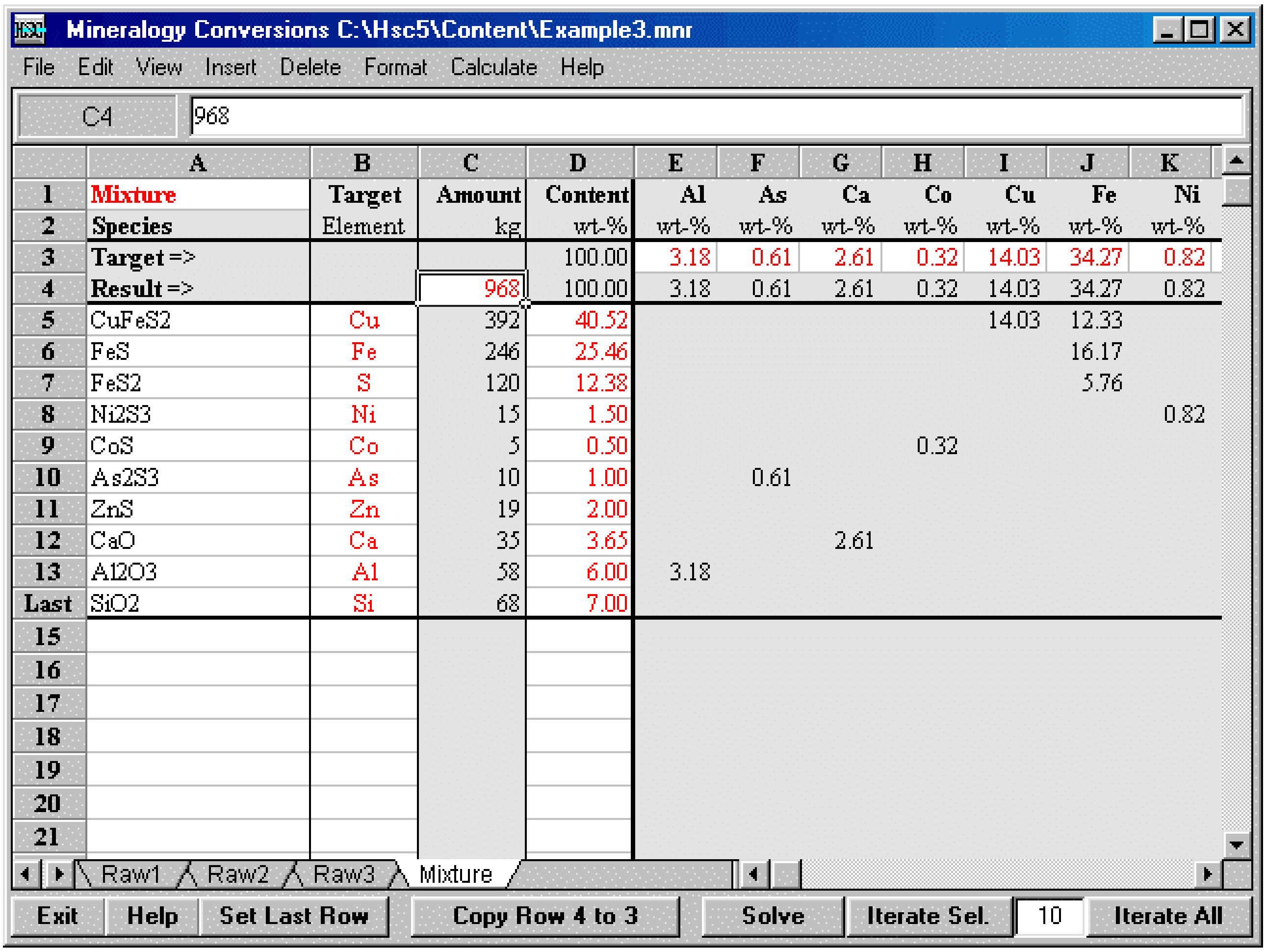
Pressing **Set Last Row** will set the last row which is used in the calculations. All compositions below this row are kept constant. This property can be used, for example, if the contents of some species, such as SiO_2, Al_2O_3, etc., are available.

Calculate Mixture Composition

The user can insert new sheets into the mineralogy workbook with the **Insert Sheet** selection. This will create an identical sheet on the right side of the selected sheet. The new sheet can be cleared with the **Edit Clear All** selection. These identical sheets may also be used for mixture calculations.

Quite often the feed of a chemical process consists of several raw materials. The compositions of these materials are fixed, but the ratios change from time to time. The total composition of the mixture may be calculated with the Mineralogy module and by following these steps, see Fig. 5 (file name of this example is **Example3.mnr**):

1. Start from Example 2, shown in Fig. 4 and Select **Insert Sheet**.
2. Double click the sheet 1 tab and rename the sheet as Raw1. Rename sheet 2 in the same way as Raw2, you can also use real names for the materials.
3. Type or solve the compositions for each individual sheet as described before in this chapter. Do not add or remove species from the list, the species list must be identical in each sheet. Give the amounts for each material in the C4 cells.
4. Select **Calculate Mixture Composition**. This will add a mixture sheet and calculate the mixture composition for all the raw materials and give the total amount of the feed in cell C4.



	A	B	C	D	E	F	G	H	I	J	K
1	Mixture	Target	Amount	Content	Al	As	Ca	Co	Cu	Fe	Ni
2	Species	Element	kg	wt-%	wt-%	wt-%	wt-%	wt-%	wt-%	wt-%	wt-%
3	Target =>			100.00	3.18	0.61	2.61	0.32	14.03	34.27	0.82
4	Result =>		968	100.00	3.18	0.61	2.61	0.32	14.03	34.27	0.82
5	CuFeS2	Cu	392	40.52					14.03	12.33	
6	FeS	Fe	246	25.46						16.17	
7	FeS2	S	120	12.38						5.76	
8	Ni2S3	Ni	15	1.50							0.82
9	CoS	Co	5	0.50				0.32			
10	As2S3	As	10	1.00		0.61					
11	ZnS	Zn	19	2.00							
12	CaO	Ca	35	3.65			2.61				
13	Al2O3	Al	58	6.00	3.18						
Last	SiO2	Si	68	7.00							
15											
16											
17											
18											
19											
20											
21											

Fig. 5. Calculation of the mixture composition of three raw materials.

Copy Row 4 to 3

This button will copy all the elemental composition values from row 4 to row 3.

Number of Iterations

The default number of iterations is 10, but it can be changed in the cell left of the **Iterate All** button. The program carries out a maximum of 10 iterations each time **Iterate All** is pressed. You can decrease the number of necessary iterations by giving some preliminary guess values into column D. *In some cases preliminary guess values are needed to help the iteration routine to find the correct answer*.

Other Properties

The same type of formatting properties as in other HSC modules are available, such as **Format Number**, **Insert Row**, **Edit Copy**, etc.

The user can also save the workbook for later use by selecting **File Save** and read it back with the **File Open** selection. It is recommended to save the files quite often with different names such as Feed1, Feed2, etc. in order to recover the original settings in case of mistakes. The files can also be saved and opened using Excel 5 format.