

PRISMA

Application Note #1: Using IonConc and ColorComposer

1. Introduction

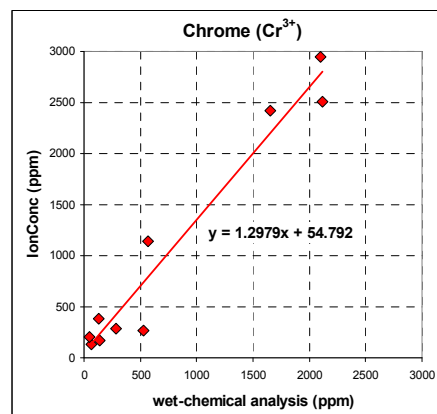
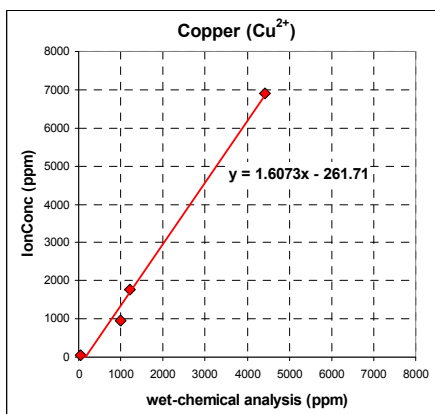
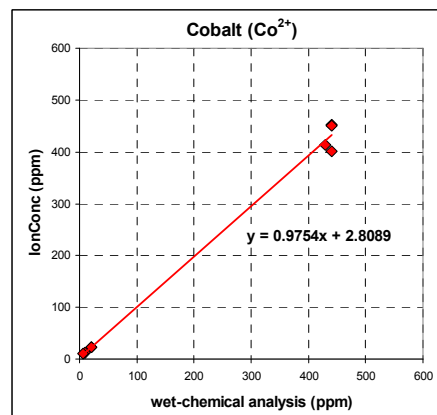
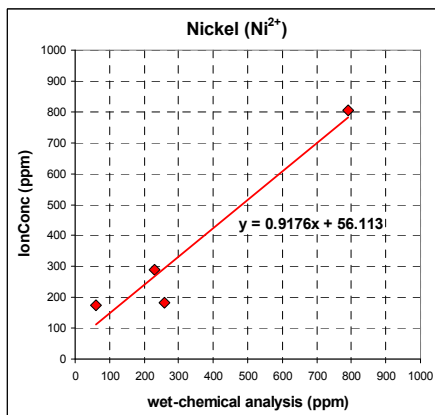
With PRISMA, the IonConc module determines the absolute concentrations of important coloring ions (currently Fe^{2+} , Ni^{2+} , Co^{2+} , Cu^{2+} , Cr^{3+} and Mn^{3+}) in soda-lime-silica glass directly from the measured transmittance spectrum. Contrary to conventional methods, IonConc not only considers individual spectral lines but processes the whole visible spectrum.

The ColorComposer module reverses the IonConc approach and calculates the transmittance spectrum and the color effect of oxide-colored soda-lime-silica glass from given ion concentrations (currently $\text{Fe}^{2+/3+}$, $\text{Cr}^{3+/6+}$, Cu^{2+} , Co^{2+} , Ni^{2+} and Mn^{3+}).

2. Procedure

To calculate the absolute concentration of ions in soda-lime-silica glass with IonConc a calibration function is needed, for example, obtained from wet-chemical analysis. The concentrations are determined with a suitable analytical method and then compared with the results calculated with IonConc (without calibration).

As an example, the following figure shows this comparison for some packaging glass samples. The results from the wet-chemical analysis are plotted against the x-axis. The results from the IonConc calculation (without calibration) are plotted against the y-axis. A regression line for all values can be calculated by using, for example, Microsoft Excel.

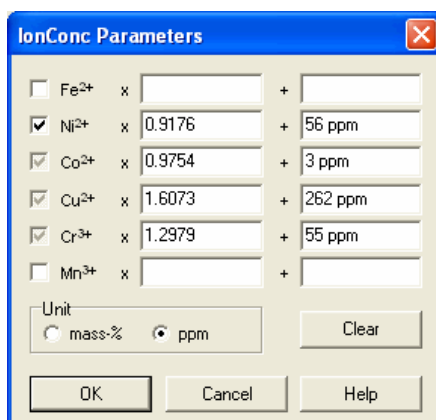


The parameters **a** and **b** in the computed regression functions $y = a * x + b$ can be directly transferred to the "IonConc Parameters" dialog box (see below). Using these calibration parameters, the calculation of the absolute ion concentrations in IonConc delivers realistic results.

3. Parameters and Calibration of IonConc

In order to obtain reliable calculation results, it is first necessary to calibrate IonConc. This is done by defining which ion types exist in the glass and entering calibration parameters for these ions. Because this information depends on the glass type and glass color, these settings are stored in the measuring template.

The following figure shows the "IonConc Parameter" dialog box, where you enter the calibration parameters. The dialog box is opened by pressing the "Edit..." button on the "Options" tab card of the measuring template.



The first task is to specify which ion types exist in the glass:

- Activate the checkboxes of all ion types that definitely exist in the glass (in the example Ni²⁺).
- Deactivate the checkboxes of all ion types that definitely do not exist in the glass (in the example Mn³⁺ and Fe²⁺).
- Gray the checkboxes for all ion types that may be found in the glass. If these ions definitely exist in the glass, click the checkboxes again to activate them.

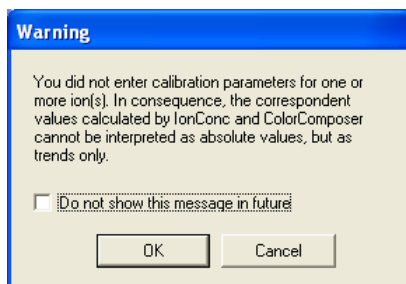
For grayed ions types IonConc automatically calculates the combination that leads to the best correlation coefficient (see section 4).

Important: Incorrect entries in this dialog lead to misinterpretations and calculation errors of the ion concentrations in the glass, such as negative results. You can verify the settings by using the plausibility check function in PRISMA (see section 5).

The second task is to enter the calibration parameters for each ion type that is either checked (definitely exists in the glass) or grayed (may exist in the glass):

- In the "Unit" field select if the calibration parameters are entered in ppm or in mass-%.
- Enter a factor in the input field next to the "x" character (parameter **a** of the regression function). The results for the corresponding ion will be multiplied by this factor.
- Enter an addend in the input field next to the "+" character (parameter **b** of the regression function). After multiplication, this value will be added to (or subtracted from if negative) the results for the corresponding ion.

IonConc can also be used without calibration, for example, to perform trend analyses without absolute information. Activate the checkboxes of the desired ions as described above, without entering the calibration parameters. When you close the dialog box by clicking the "OK" button, a warning message appears which can be accepted by clicking "OK" again.



4. Result Presentation

After the measurement of a sample, the computed concentration values are displayed on the "IonConc" tab card in the "Redox Analysis" diagram window (see following figure).

- Fe2+** Fe²⁺ concentration in mass-% Fe₂O₃
- Ni2+** Ni²⁺ concentration in mass-% NiO
- Co2+** Co²⁺ concentration in mass-% CoO
- Cu2+** Cu²⁺ concentration in mass-% CuO
- Cr3+** Cr³⁺ concentration in mass-% Cr₂O₃
- Mn3+** Mn³⁺ concentration in mass-% MnO

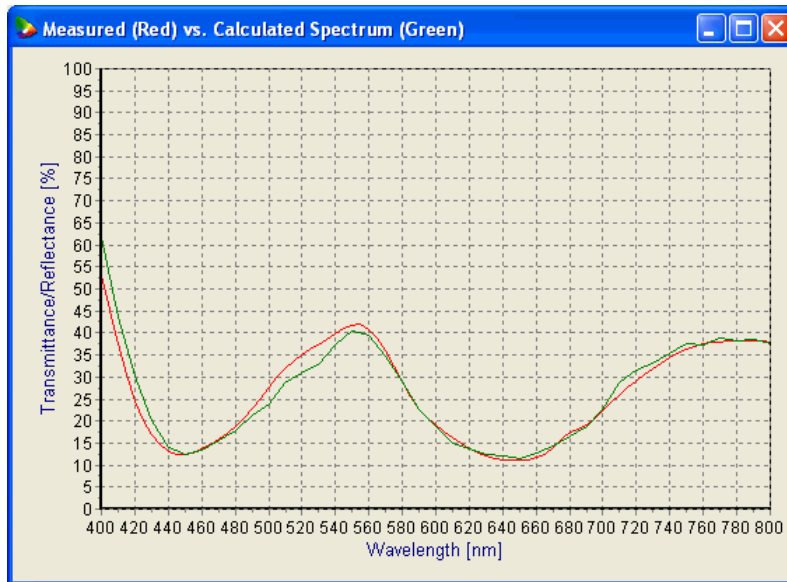
Date/Time	Name	r	Fe2+	Ni2+	Co2+	Cu2+	Cr3+	Mn3+
8/6/2001 6:42 PM	Green glass A	0.9751		0.0266 %			0.2147 %	
8/6/2001 6:42 PM	Green glass B	0.9758		0.0879 %	0.0165 %		0.3628 %	
8/6/2001 7:09 PM	Flint glass C	0.9868		0.0026 %			0.0006 %	
8/6/2001 7:14 PM	Flint glass D	0.9605		0.0045 %				

The values are listed in mass-% in relation to the corresponding oxide (for example, Fe₂O₃ for Fe²⁺). Please note that results are computed for only those ions that are in the checked or grayed state in the "IonConc Parameters" dialog box.

The correlation coefficient r indicates the congruence of the calculated and the measured spectrum (see following section). If the correlation coefficient has the value 1, the spectra are identical.

5. Plausibility Check

You can check the plausibility of the results by selecting "Calculate Spectrum" in the drop-down menu of a row of data. This reverses the process and calculates a transmittance spectrum from the determined concentration, which you can then compare to the actually measured spectrum, as shown in the following figure:



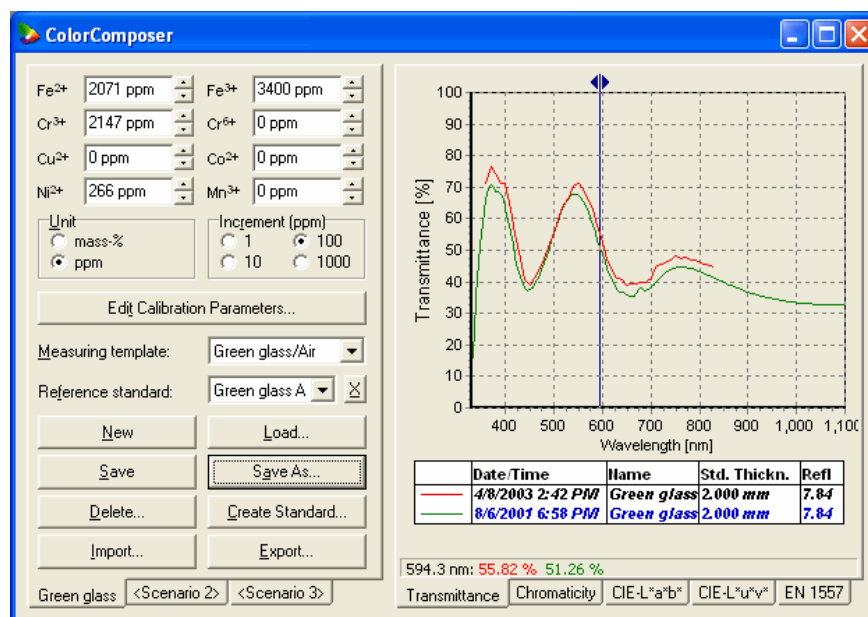
If the spectra differ significantly, either the calibration parameters are incorrect or the concentration calculation failed for the analyzed sample. The latter case could be due to chromophores that are not detected and supported by IonConc. At present, this applies in particular to the amber chromophore (FeS) and selenium compounds (Se⁰, FeSe).

You can try out different parameter combinations for the current measurement in the "IonConc Parameters" dialog box, which you open by selecting "Parameters..." from the drop-down menu of the row of data. Here you can change the settings as described in section 3. When you click "OK", the results for the selected row are updated according to the new parameters.

6. ColorComposer

The ColorComposer module reverses the IonConc approach and predicts the transmittance spectrum and the color values from given ion concentrations.

The following figure shows the ColorComposer window, which opens by selecting "ColorComposer..." in the "Prisma" menu or by clicking the corresponding toolbar button.



This window consists of two parts: the left side, which lets you set the parameters, and the right side, which displays the results. On the left side, you enter the concentrations of coloring ions in mass-% or ppm and select the measuring template from which the parameters for the simulation should be taken. (By default, the first measuring template in the list is chosen.)

You can compare different parameter combinations by switching between the three tab cards on the left (" $<$ Scenario 1 $>$ " to " $<$ Scenario 3 $>$ "). After you have saved a scenario, the tab will be labeled with the entered name, like "Green glass" in the above screenshot.

After you modify a concentration value, the diagram on the right side is automatically updated. The tabs at the bottom allow you to toggle between the transmittance spectrum, the chromaticity diagram and the $L^*a^*b^*$ or $L^*u^*v^*$ color spaces.

To display the monitor color effect of the simulated sample, select the "Properties" entry from the drop-down menu of the row of data.

You can enter your own calibration parameters in the ColorComposer or adopt the parameters defined in the measuring template to simulate the effect of different ion concentrations. To enter calibration parameters, click the "Edit Calibration Parameters" button. The "IonConc Parameters" dialog box opens. Because the ColorComposer allows the ions Fe^{3+} and Cr^{6+} in addition to the ions in IonConc, the dialog looks different from the dialog opened from the measuring template:

Ion	Concentration	Unit
Fe^{2+}		
Fe^{3+}		
Ni^{2+}	0.9176	56 ppm
Co^{2+}	0.9754	3 ppm
Cu^{2+}	1.6073	262 ppm
Cr^{3+}	1.2979	55 ppm
Cr^{6+}		
Mn^{2+}		

Unit: mass-% ppm

If you want to adopt the parameters defined in the measuring template, click the "Copy Parameters From Template" button.

By using the determined calibration parameters, the simulated spectra and the color values are calculated realistically in the ColorComposer.

Important: The ColorComposer demonstrates the color effect of various ion combinations for informative and educational purposes only. There is no guarantee or warranty that the actual color values of the glass agree with the prediction generated by this tool. In particular, the IonConc calibration parameters entered in the measuring template above are only examples and can not be used for measuring real samples.