The following appears as a link in the website "Paper Through Time—Non-destructive Analysis of 14^{th}-19th Century Papers," T. Barrett et al, under the DISCUSSION section. http://paper.lib.uiowa.edu/chron.php.

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Calculating Weight Percent Calcium Carbonate, Potash Alum, and Papermaker's Alum Present in Paper from Parts per Million Figures Determined by X-Ray Fluorescence Spectrometry

1. For all papers tested in this study: Weight percent calcium carbonate (wt% $CaCO_3$) from parts per million calcium (ppm Ca)

Assumptions

- All calcium in the sheet was introduced as $CaCO_3$.
- None of the $CaCO_3$ has subsequently been lost due to ion exchange, meaning that there is no change in $CaCO_3$ concentration due to the bonding of the Ca^{2+} cations with anions other than CO_3^{2-} to form different salts. A reasonable assumption given the poor solubility of $CaCO_3$ in water at neutral pH.

Given

$$y \text{ ppm Ca} = \frac{y \text{ g Ca}}{10^6 \text{ g total substance}}$$

Multiplying the expression on the right by one four times

$$\times \frac{1 \text{ mol Ca}}{40.078 \text{ g Ca}} \times \frac{1 \text{ mol CaCO}_3}{1 \text{ mol Ca}} \times \frac{100.087 \text{ g CaCO}_3}{1 \text{ mol CaCO}_3} \times \frac{10^{-4}}{10^{-4}}$$

equals

$$\frac{2.497 \times 10^{-4} y \text{ g CaCO}_3}{10^2 \text{ g total substance}} = 2.497 \times 10^{-4} y \text{ wt\% CaCO}_3$$

wt% $CaCO_3$ = 0.0002497 * (ppm Ca)

2. Wt% potash alum (aluminum potassium sulfate dodecahydrate, $AlK(SO_4)_2 \bullet 12H_2O$) from ppm potassium (K) for papers dated before 1800 (specimens 1361-001 through 1799-005)

Assumptions

- All potassium in the sheet was introduced as potash alum that had 12 water molecules per potassium atom in its crystal structure ($AlK(SO_4)_2 \bullet 12H_2O$), which is the commonest hydrate.
- There has been no conversion of $AlK(SO_4)_2 \bullet 12H_2O$ to other salts/complexes during or after papermaking. Only a fair assumption, given the ability of the aluminum(III) cation to exchange ligands within the sheet.
- The water molecules that were present in the potash alum crystals remain present in the sheet.

Given

$$y \text{ ppm K} = \frac{y \text{ g K}}{10^6 \text{ g total substance}}$$

Multiplying the expression on the right by one four times

$$\times \frac{1 \text{ mol K}}{39.0983 \text{ g K}} \times \frac{1 \text{ mol AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}}{1 \text{ mol K}} \times \frac{474.39 \text{ g AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}}{1 \text{ mol AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}} \times \frac{10^{-4}}{10^{-4}}$$

equals

$$\frac{1.213 \times 10^{-3} y \text{ g AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}}{10^2 \text{ g total substance}} = 1.213 \times 10^{-3} y \text{ wt\% AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}$$

wt% $AlK(SO_4)_2 \bullet 12H_2O$ = 0.001213 * (ppm K)

3. Wt% potash alum from ppm sulfur (S) for papers dated before 1800 (specimens 1361-001 through 1799-005)

Assumptions

- All sulfur was introduced as $AlK(SO_4)_2 \bullet 12H_2O$.
- There has been no conversion of $AlK(SO_4)_2 \bullet 12H_2O$ to other salts/complexes during or after papermaking.
- The water molecules that were present in the potash alum crystals remain present in the sheet.

Given

$$y \text{ ppm S} = \frac{y \text{ g S}}{10^6 \text{ g total substance}}$$

Multiplying the expression on the right by one four times

$$\times \frac{1 \text{ mol S}}{32.066 \text{ g S}} \times \frac{1 \text{ mol AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}}{2 \text{ mol S}} \times \frac{474.39 \text{ g AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}}{1 \text{ mol AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}} \times \frac{10^{-4}}{10^{-4}}$$

equals

$$\frac{7.397 \times 10^{-4} y \text{ g AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}}{10^2 \text{ g total substance}} = 7.397 \times 10^{-4} y \text{ wt\% AlK(SO}_4)_2 \bullet 12\text{H}_2\text{O}$$

wt% $AlK(SO_4)_2 \bullet 12H_2O$ = 0.0007397 * (ppm S)

4. Wt% papermaker's alum $Al_2(SO_4)_3 \bullet 17H_2O$ (aluminum sulfate heptadecahydrate) from ppm S for papers from 1800 and after (specimens 1801-001 through 1899-002)

Assumptions

- All sulfur was introduced to the paper as aluminum sulfate heptadecahydrate. This is certain to be false, but the resulting calculation represents an average between the two commonest hydrates, aluminum sulfate hexadecahydrate ($Al_2(SO_4)_3 \bullet 16H_2O$) and octadecahydrate ($Al_2(SO_4)_3 \bullet 18H_2O$).
- There has been no conversion of $Al_2(SO_4)_3 \bullet 17H_2O$ to other salts/complexes during or after papermaking. Again, only a fair assumption given the expected ligand exchange around aluminum(III).
- The water molecules that were present in the papermaker's alum crystals remain present in the sheet.

Given

$$y \text{ ppm S} = \frac{y \text{ g S}}{10^6 \text{ g total substance}}$$

Multiplying the expression on the right by one four times

$$\times \frac{1 \text{ mol S}}{32.066 \text{ g S}} \times \frac{1 \text{ mol Al}_2(\text{SO}_4)_3 \bullet 16\text{H}_2\text{O}}{3 \text{ mol S}} \times \frac{648.385 \text{ g Al}_2(\text{SO}_4)_3 \bullet 17\text{H}_2\text{O}}{1 \text{ mol Al}_2(\text{SO}_4)_3 \bullet 17\text{H}_2\text{O}} \times \frac{10^{-4}}{10^{-4}}$$

equals

$$\frac{6.740 \times 10^{-4} y \text{ g Al}_2(\text{SO}_4)_3 \bullet 17\text{H}_2\text{O}}{10^2 \text{ g total substance}} = 6.740 \times 10^{-4} y \text{ wt\% Al}_2(\text{SO}_4)_3 \bullet 17\text{H}_2\text{O}$$

wt% $Al_2(SO_4)_3 \bullet 17H_2O$ = 0.0006740 * (ppm S)