

CHEMICAL NOTATION USING T<sub>E</sub>X

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The article below, from a mineralogy handbook, illustrates the fact that publishing in disciplines other than mathematics and computer science can benefit from the use of T<sub>E</sub>X. A few changes were necessary to fit the copy into TUGboat's narrow columns: the bar chart was truncated at 7.5cm (10cm in the original), and some line breaks and spacing were indicated manually where the appearance of the copy would otherwise have been less than desirable (the original column width was 3.5in, the TUGboat column width, 18.75pc = 3.125in, just enough of a difference to be troublesome).

The tables are built with ordinary `\halign` coding; especially attractive is the centering of headings over multiple columns in the table following *Powd. Pat.* The most interesting control sequences defined for this document are for the chemical formulas and the bar chart:

*Chemical formula:*

```
\def \F#1 {\if A\whatptsize
  {\mathsy uzz\mathit adf $#1$}}
\else{\if 9\whatptsize
  {\mathsy vzz\mathit bef $#1$}}
\else{\if 8\whatptsize
  {\mathsy wzz\mathit cef $#1$}}
\else{}}}
```

This macro depends on the definition within the `\dotspoint` macros (cf. `basic.tex`) of a control sequence `\whatptsize` which allows the current size to be tested; single-digit sizes are represented by one digit, and larger sizes follow the example of hexadecimal notation ( $A = 10$ , etc.). Notice that subscripts are defined to be the same size, regardless of level, and roman fonts are substituted for the usual math italic to simplify typing. Double braces ensure locality of these substitutions.

*Bar chart:*

```
\def\1{\hbox to 5mm
  {\hfill\vrule depth 3pt}}
\def\2{\hbox to 5mm
  {\hfill\vrule depth 5pt}}
\def\#1 #2 {\hbox to #1mm
  {\hfill\vrule height #2pt}}
```

All dimensions in the original were true, but since the AMS version of T<sub>E</sub>X doesn't yet support that feature, they were replaced by ordinary dimensions.

The input looks like this:

```
\vbox{\hbox to 7.5cm{\vrule height 5pt
\e 10.09 4
\l 1.74 3
\l 4.25 9
\l 0.38 3
} %end of hbox
\hrule
\hbox to 7.5cm{\vrule depth 8pt
\1\2\1\2\1\2\1\2\1\2\1\2\1\2\1\2\1
\hss} %end of hbox
\vskip 1pt
\hbox to 7.5cm{\eightpoint
American Mineralogist {\bf 55}, 1100,
(1970)}\hfill$2\theta\toright$}
} %end of vbox
```

The `\hss` following the `\1\2...` line is used to an overfull box exactly the width of the last `\v`.

And finally, here is the article we've been talking about.

HEMIHEDRITE  $\text{ZnF}_2\{\text{Pb}_5(\text{CrO}_4)_3\text{Si}$

Morph. Triclinic-Pedial, 1;  $C_1$

**Habit.** Well-formed doubly-terminated crystals from 0.2 to 10 mm in length. Elongated parallel to [001] with 80 forms reported. Twins most commonly by reflection in  $\bar{2}23$  as penetrations of crystals of opposite hand to form an X, V, or Y shape with inclined at  $B^\circ$ . Less commonly by reflection in  $0\bar{1}2$ , also by reflection in  $0\bar{1}2$ .

**Phys.**  $H = 3$ ;  $\rho_{meas} = 6.42$ ;  $\rho_{calc} =$  poor cleavage on {110}. Color bright orange to henna brown to almost black. Streak saffron yellow (Munsell 5Y8/10).

**Struct.**<sup>2</sup> The structure is similar to those of the tsumebite series and contains a Zn coordinated to four O and two F; the Pb environments are varied. Cr and Si are regularly four-coordinated to O.

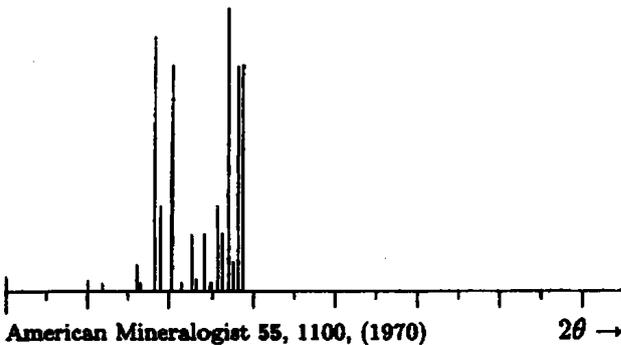
**Occur.** In a secondary oxide vein assemblage suggestive of alkaline solutions of relatively low pH. Associated with cerussite, wulfenite, vauquelinite, willemite, and mimetite. Primary minerals include galena, pyrite, and tennantite.

**Distr.** Known only from two Arizona localities. The type locality is the Florence Lead-Silver Mine, Pinal County; also at the Rat Tail Claims, near Winkelman, Maricopa County.

**Name.** For its distinct hemihedral morphology.

Ref.

1. Williams, S. A. and Anthony, J. W. (1970), Hemihedrite, A New Mineral From Arizona, *Am. Min.* 55, 1088-1102.
2. McLean, W. J. and Anthony, J. W. (1970), The Crystal Structure of Hemihedrite, *Am. Min.* 55, 1103-1114.



Powd. Pat. Debye-Scherrer (114.6 mm; CuK $\alpha_1$ ; Visual I).

STRONGEST LINES		LARGEST <i>d</i> SPACINGS					
3.301	100	8.765	4	4.364	80	3.478	30
4.872	90	7.481	3	4.136	3	3.399	20
4.364	80	5.512	9	3.909	20	3.301	100
3.164	80	5.384	3	3.820	4	3.234	10
3.102	80	4.972	90	3.676	20	3.164	80
2.924	55	4.675	30	3.584	3	3.102	80

Struct. Cell.  $P1 - C_1^1$ ;  $Z = 1$ ;

$$a = 9.497(1), \quad b = 11.443(2), \quad c = 10.841(2)$$

$$\alpha = 120^\circ 30(1)', \quad \beta = 92^\circ 06(1)', \quad \gamma = 55^\circ 50(1)'$$

$$a : b : c = 0.830 : 1 : 0.947$$

Chem. Substitution of Zn for Pb noted in some samples.

	1	2
ZnO	2.7	3.93
PbO	73.0	70.5
Cr <sub>2</sub> O <sub>3</sub>	19.7	19.5
SiO <sub>2</sub>	3.9	3.2
F	1.2	5.1
-O $\equiv$ F	-0.5	-2.1
Total	100.0	100.0

1. ZnF<sub>2</sub>[Pb<sub>5</sub>(CrO<sub>4</sub>)<sub>3</sub>SiO<sub>4</sub>]<sub>2</sub>.
2. Average of several partial analyses.

Opt. Thin section shows feeble pleochroism with  $Z > Y > X$ . Relief extreme; dispersion resembles horizontal dispersion.

$$\alpha = 2.105(5) \text{ yellow} \quad (2V_z)_{meas} = 92^\circ(-)$$

$$\beta = 2.32(2) \text{ yellow} \quad (2V_z)_{calc} = 88^\circ(+)$$

$$\gamma = 2.65(2) \text{ orange}$$

\* \* \* \* \*

Problems

\* \* \* \* \*

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Balancing Columns of Text and Translation

In the last issue, Johnny Stovall asked about a macro that could adjust the width of each column of two-column output so that the lengths of the two columns will be equal. His application involves typesetting original texts in parallel with translations. As long as reliable estimates of the relative length of the two segments are available, a simple technique can be used. `\varunit` can be set to the width available for text in both columns (excluding margins), and the actual width of each column can then be set in terms of a percentage of `vu`.

The following macro illustrates this approach using `\hbox` par:

```
\input basic
\varunit 6in % Space available for both
              % columns, exclusive of margins
\def\intercolumnspacing{\hskip .5in}
% Arguments to \trans are percentages
% of total width for first column,
% contents of first column, percentage
% of total width for second column, and
% contents of second column, respectively.
% The two numbers should sum to 100.
\def\trans#1#2#3#4{
  \hbox{\hbox par 0.#1vu
        {#2}\intercolumnspacing
        \hbox par 0.#3vu{#4}}
}
```

Here is a simple example:

Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party.	Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party. Now is the time for all good men to come to the aid of their party.
--	--

And continue ...

Here, it is assumed that there is text extending across the full page width above or below the translations. This macro must be modified if the text segments include multiple paragraphs. A similar macro