

Use of the BATCH Number with Hand-Manipulated Files

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The use of a simple, structural-atomic code for organic compounds, the BATCH Number, is described in the nonmachine management of card and document files.

The five-digit, structural-atomic code, the BATCH Number, has been introduced for the machine management of information on organic compounds (1). The BATCH Number and similarly based, easily mastered classification codes should also be of value in hand-managed applications. It is the purpose of this paper to report two studies in this domain.

APPLICATION OF THE BATCH NUMBER TO CARD FILES

Where information on individual organic compounds is presented on file cards, retrieval operations can be expedited by recording and filing the cards according to the BATCH Number. Conventionally, such cards would be filed by either the chemical name or molecular formula. The success of the former arrangement is limited by the variety of chemical names assigned offhand by different workers or even by the same worker at different times. The use of the molecular formula is limited by the low degree of discrimination with respect to chemical groups.

In the trial experiment, a file of over 5000 cards, each showing an assigned name, structural formula, molecular formula, and additional chemical and commercial data, was employed. It was found that the BATCH Number could be assigned accurately by a chemically-oriented clerk after a preliminary handsort by the chemist according to the value of the B-digit. The cards were then filed according to the BATCH Number, treated as a conventional five-digit number.

Previous experience indicated that the resulting file could be handled more readily by the introduction of color coding for the B, A, and T-digits. Such coding of hand files has been expedited in recent years by the availability of inexpensive, colored-ink markers. Liquid inks are to be preferred because, as the result of diffusion, the color is made visible on the face of the cards. The scheme shown in Figure 1 was found appropriate. The arrangement of the stripes allows visual recognition of singular and plural measures implicit in the scheme for the assignment of the BATCH Number (1).

The B and A-digit values are coded as color stripes at the left and right, respectively, of the top edge of the cards. The colors assigned the B-digit are in their spectral order. The colors employed for the A-digit have some mnemonic or phonetic association with the atomic classes. The T-digit is assigned as an appropriately placed

black stripe on the edge of the right side of the card. An *uncommitted* digit value, which is indicated by a hyphen in the BATCH Number (1), is left *uncolored*—that is, without a stripe. The maximum width allowed for a stripe obviously depends on the card size. Positioning of the stripes need not be exact and can be accomplished freehand by comparison with a "scheme" card, such as that shown in Figure 1.

In the machine use of the BATCH Number, listings by both BA divisions and AT divisions provide BATCH Directories for desk use in the retrieval of compounds of interest (1, 2). Color coding facilitates the analogous use of a hand file. BA divisions may be recognized immediately by inspection of the stripes on the top edge of the cards. If the cards corresponding to the BA divisions of interest are turned up in the file with their right edge upward, associated values of the T-digit are then fully displayed. A search by AT divisions is accomplished by turning up the cards in the A divisions of interest and then turning down the cards in the T divisions *not* of interest.

Since the left and bottom edges of the cards are unused, they can be employed for other simple visual codes.

Obviously, the BATCH Number might be used with edge-notched cards employing a numerical field for each of the digits of the BATCH Number or for the B, A, and T-digits only. However, this application would require more input time than the simple "gang" striping of packs of cards and, consequently, has not been investigated.

APPLICATION OF THE BATCH NUMBER TO DOCUMENT FILING

The BATCH Number also has been employed effectively for the initial organization of a document file related to organic compounds. This application is promising even where documents differing in size, content, and character—e.g., letters, data sheets, brochures, and memoranda—must be correlated and retrieved with a minimum of total effort. Where a document file of possibly up to several thousand items is involved, it is feasible to employ only the B, A, and T-digits of the BATCH Number as file headings. Indeed, where only the B and A-digits are used, these two values usually can be assigned by the chemist from the chemical name in the document without having the actual structure or molecular formula in view.

| | | | | | | | | | | | | | | | | | | | | | | | |
|---------------------------|---|---|---|---|---|---|---|---|---|-----------------------------|---|---|---|---|---|---|---|---|---|---|---|----|--|
| BK | R | R | O | O | Y | Y | G | B | P | R | P | Y | G | Y | O | G | O | G | G | G | G | BK | |
| B - DIGITS (RING CLASSES) | | | | | | | | | | A - DIGITS (ATOMIC CLASSES) | | | | | | | | | | | | | |
| 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 | 0 | | | | |

SYMBOLS FOR COLOR STRIPES:

| | |
|----|--------|
| B | Blue |
| BK | Black |
| G | Green |
| O | Orange |
| P | Purple |
| R | Red |
| Y | Yellow |

(TOTAL HETEROATOM COUNT)
 T - DIGITS

| |
|---|
| 0 |
| 1 |
| 2 |
| 3 |
| 4 |
| 5 |
| 6 |
| 7 |
| 8 |
| 9 |

Figure 1. Layout for 1/4-inch stripes on cards or sheets, IBM size (7 3/4 x 3 1/4 inch) or larger

REMARKS

Broad application of the BATCH Number (and similar easily mastered classification codes) and visual color coding to the management of unmechanized information files is suggested by the experiments described above. Where a file grows in size and/or attains a degree of permanence warranting mechanization, the conservative measures

represented by the BATCH Number can be continued without need for change.

LITERATURE CITED

- (1) Barnard, A. J., Jr., Kleppinger, C. T., Wiswesser, W. J., *J. Chem. Doc.* 6, 41 (1966).
- (2) *Ibid.*, 6, 48 (1966).

Division of Chemical Literature Program

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MONDAY MORNING AND AFTERNOON

Symposium on Compilations of Data on Chemical
and Physical Properties of Substances

G. Waddington, Presiding

- 9:00- G. Waddington. Introductory Remarks.
- 9:10- 1. F. D. Rossini. Historical Background of Current Data Compilation Activities.
- 9:40- 2. E. L. Brady. The National Standard Reference Data System (NSRDS).
- 10:00- 3. H. M. Weisman. Needs of ACS Members for Property Data.
- 10:20- 4. E. R. Johnson. NSRDS Program in Thermodynamic and Transport Properties.
- 10:50- 5. S. A. Rossmassler. NSRDS Program in Atomic and Molecular Properties.

- 11:20- 6. R. M. S. Hall. Data Compilation Activities in the United Kingdom.

E. L. Brady, Presiding

- 2:00- 7. G. Waddington. A World System of Data Compilations.
- 2:30- 8. L. Kuentzel. Organizing Physical Molecular Data for Qualitative Chemical Analysis.
- 3:00- 9. F. Y. Speight. Numerical Data Activities in Engineering Societies.
- 3:30-10. Y. S. Touloukian. The Thermophysical Properties Research Center.
- 4:00-11. D. Garvin. The NBS Chemical Kinetics Information Center.
- 4:20-12. H. Ondik, J. Donnay. Crystal Data.
- 4:40-13. A. Ross, M. Burton. The Radiation Chemistry Data Center.