

Memo 4C-3/90

28 September 1973

To: Distribution

From: H.D. Lemmel *Lemmel*

Subject: Reply to Memo 4C-1/40 (proposed codes)
Provisional Manual and LEXFOR pages on
Compounds.

Enclosure: Provisional Manual page VIII.16 dated 73-9-30
Provisional LX4 page "COMP" dated 73-9-30

Distribution: Dr. F. Fröhner, NDCC (5)
Dr. S. Pearlstein, NNGSC (5)
Dr. V. Manokhin, CJD (5)
NDS: P. M. Attree
A. Calamand
C.L. Dunford
J. Lemley
H.D. Lemmel
J.J. Schmidt
file

Clearance:
J.J. Schmidt

J.J. Schmidt

1. Re lab-code IUSALTI: This entry exists in dictionary 3 since the beginning of EXFOR.
2. Re compounds-code 40-ZR-ALY: It was agreed that new codes for special compounds "should not be introduced unless many such data can be expected". For Zircaloy this is not the case, since there is not a single CINDA entry for this material. The Exfor-entry should therefore use "40-ZR-CMP" with "ZIRCALOY" under SAMPLE.
3. For clarification I submit updated provisional Manual and Lexfor pages on the coding of compounds. These are based on earlier Manual and Lexfor entries and on memo 4C-3/34, which was agreed Oct. 71 (INDC(NDS)-41 page 10 item 32) but never properly entered in the Manuals; see 4C-3/58 bottom of page 1 and 4C-3/59 page 2. I included also some later revisions (e.g. dropping CMP from Dict.9) and applied some discretion in the splitting of the material into a Manual entry and a LEXFOR entry.
4. It is proposed that "Provisional Manual and LEXFOR pages" be filed in the Manuals until NNCSC distributes official update pages.

CMPD-QUANT

This keyword is used instead of the keyword "ISO-QUANT", when the quantity given in the DATA table refers to chemical compounds, alloys or mixtures. The format of the coded information is the same as under "ISO-QUANT" except that the A-number within the Isotope is replaced by a three character compound-code. (See Dictionary 9 for codes.)

Example: CMPD-QUANT (26-FE-CMP,TOT)

The more precise name and/or composition of the compound is given in free text under the keyword "SAMPLE".

Example: SAMPLE FE2- ϕ 3.

One of the three keywords: ISO-QUANT, NUC-QUANT, or CMPD-QUANT must be present; they are mutually exclusive.

For coding rules see LEXFOR under Compound-codes.

Compound-codes
=====

For coding chemical compounds under the keyword "CMPD-QUANT" see Manual page VIII.16 and Dictionary 9.

In general, chemical compounds under "CMPD-QUANT" are coded by combining the code "CMP" with the element number and symbol of its main component. Example: 26-FE-CMP for iron-oxide or any other iron compound. More detailed information on the compound is given under "SAMPLE". For a small number of materials of particular importance in neutron or reactor-physics, special compound-codes are used, which are included in Dictionary 9. Example: 1-H-BNZ for benzene (C₆-H₆). The intention is that codes with CMP (e.g. 100-FM-CMP) can be used without entry in Dictionary 9, but that special codes (e.g. 100-FM-OXI for Fermium oxide) should not be introduced unless many such data can be expected. Dictionary 9 is sorted according to the periodic table. Additions require 4-centers' approval.

(In CINDA, the compound-codes are entered correspondingly in the S-A field. A more precise definition of the compound is given in the comment-field.)

Three rules must be kept in mind:

1. A more specific code has priority over a more general code.

Examples: a. Zirconium-hydrides are to be entered as 40-ZR-HYD and not as 1-H-CMP nor 40-ZR-CMP.

b. Water is to be coded as 1-H-WTR and not as 1-H-CMP.

2. For alloys (or other mixtures) the code "CMP" is to be combined with the element symbol of the major component, usually the one named first. For chemical compounds the code "CMP" is to be combined with the symbol of the primary element, usually the first one of the formula: CaCO₃ is to be coded as 20-CA-CMP, and not as 6-C-CMP or 8-O-CMP.

3. If the compiler feels that two possible codes are equally relevant, the Iso-quant combination using the equal-sign shall be used.

Examples: a. Ammonium-hydrocarbon
((7-N-AMM, TØT)=(1-H-CXX, TØT))

b. brass, if it contains 50% Cu and 50% Sn
((29-CU-CMP, TØT)=(50-Sn-CMP, TØT))

(In such cases two Cinda-entries are made, one for each Cmpd-quant.)

Typical data to be entered under "CMPD-QUANT" are low-energy data, where chemical or crystalline binding forces affect the neutron cross-sections; a typical example is the total cross-section or thermal-scattering data of H₂O. However, thermal scattering data for H₂ must be entered under "ISO-QUANT" for the isotope 1-H-1, supplemented by an entry under "SAMPLE". If for example the sample was a compound, e.g. PuO₂, and if the data given refer to Pu only, then the "ISO-QUANT" must be given and not the "CMPD-QUANT".