Coding of Chemical Compounds: Clarifications

- Memo **4C-4/113** (attached) proposes several new entries for EXFOR dictionary 9 (Compounds) and DANIEL dictionary 27 (which contains both Nuclides and Compounds), all with -CMP or -OXI as compound identifier.
- We want to clarify 2 questions:
  - What codes need to be entered in dictionary 9? (-CMP should not be needed!)
  - Should all oxides get a compound code -OXI? (We believe not).

- The EXFOR Systems Manual (page 6.7) says:

  "**Dictionary 9: Chemical Compounds.** (Codes are also used in CINDA). The general compound code CMP can be combined with any element in the form (Z-S-CMP) **without entry in this dictionary**, which only lists special cases…."

  DANIEL dictionary 27, on the other hand, does have the codes -CMP for (almost) all elements, and for some years they now appear also in EXFOR dictionary 9 (because they are both derived from the archive dictionaries). Anyway, all check programs should accept compounds with -CMP independently of an entry the dictionary.

- The LEXFOR page on Chemical Compounds says:

  "In general, chemical compounds are coded under the keyword REACTION by combing the code CMP with the element number and symbol of its main component, e.g. **26-FE-CMP for iron oxide** or any other iron compound. For a **small number of materials of particular importance for users of nuclear reaction data, special compound codes are used.** These are listed in Dictionary 9."

From this I conclude that **not** all oxides should get a special compound code, 26-FE-COMP is even mentioned as the coding for iron oxide. New compound codes should be restricted to very important special cases. (The DANIEL dictionary 27 has many -OXI codes with status INT, i.e. not for EXFOR use - why?)

Or should we change the policy on compounds and introduce codes for all oxides (when there are data) and many other compounds?

Reminder: compound codes are to be used only for certain types of low energy data; otherwise the chemical composition of the sample is given only under SAMPLE. LEXFOR says: "Typical data on compounds entered are low-energy data, where chemical or crystalline binding forces affect the neutron cross sections; an example is the total cross section or thermal-scattering data of water…"

RUSSIA'S NUCLEAR DATA CENTER - RNDC
Alias: CENTR JADERNYKH DANNYKH - CJD
Bondarenko Sq., 1
Institute of Physics and Power Engineering - IPPE
Obninsk 249020
Kaluga Region, RUSSIA

(*Internet*) manokhin@ippe.obninsk.ru Telephone: (+7 08439)989-82
FAX: (+7 095)883-3112

MEMO 4C-4/113

DATE: 18 Dec 2000
TO: Distribution
From: S. Maev (alias: S.Mayev)
Subject: Exfor Dictionary 09 and Daniel Dictionary 27 update

Exfor Dictionary 9 (Compounds)

67-HO-CMP Holmium compound
67-HO-OXI Holmium oxide

Daniel Dictionary 27

```
 27 PRO 2000nn  27-CO-CMP          COCMP nnnnn1 3      C
                                                        COBALT COMPOUND
 27 PRO 2000nn  27-CO-OXI          COOXI nnnnn1 3      C
                                                        COBALT oxide
 27 PRO 2000nn  50-SN-OXI          SNOXI nnnnn1 3      C
                                                        TIN  oxide
 27 PRO 2000nn  65-TB-CMP          TBCMP nnnnn1 3      C
                                                        TERBIUM compound
 27 PRO 2000nn  65-TB-OXI          TBOXI nnnnn1 3      C
                                                        TERBIUM oxide
 27 PRO 2000nn  67-HO-CMP          HOCMP nnnnn1 3      C
                                                        HOLMIUM COMPOUND
 27 PRO 2000nn  67-HO-OXI          HOOXI nnnnn1 3      C
                                                        HOLMIUM oxide
 27 PRO 2000nn  68-ER-CMP          ERCMP nnnnn1 3      C
                                                        ERBIUM COMPOUND
 27 PRO 2000nn  68-ER-OXI          EROXI nnnnn1 3      C
                                                        ERBIUM oxide
```

==========

EXPLANATION

While compiling data for ultra-cold neutrons coherent scattering I met the necessity to use as targets anf residual neclei oxides and compounds. After running CHEX program this results in following error messages (records are split in two parts):

```
 ENTRY 22450,
 -----------
     REFERENCE  (J,ZP/A,357,297,1997)
```

```
  Illegal use of nuclide                  field  4
  REACTION   (65-TB-CMP(N,THS)65-TB-CMP,COH,AMP)Coherent Scattering
                              ^^^^^^^^^                                  22450  200003
-------------------------------------------------------------------
 Illegal use of nuclide                   field  4
  REACTION   (65-TB-OXI(N,THS)65-TB-OXI,COH,AMP)Coherent Scattering
                              ^^^^^^^^^                                  22450  300003
-------------------------------------------------------------------
 Illegal code in                          field  1
 Illegal code in                          field  4
  REACTION   (67-HO-CMP(N,THS)67-HO-CMP,COH,AMP)Coherent Scattering
              ^^^^^^^^^       ^^^^^^^^^                                  22450  500003
-------------------------------------------------------------------
 Missing independent variable             NUCLIDE                       22450  5
-------------------------------------------------------------------
 Illegal code in                          field  1
 Illegal code in                          field  4
  REACTION   (67-HO-OXI(N,THS)67-HO-OXI,COH,AMP) Coherent Scattering
              ^^^^^^^^^       ^^^^^^^^^                                  22450  600003
-------------------------------------------------------------------
 Missing independent variable             NUCLIDE                       22450  6
-------------------------------------------------------------------
 Illegal use of nuclide                   field  4
  REACTION   (68-ER-CMP(N,THS)68-ER-CMP,COH,AMP) Coherent Scattering
                              ^^^^^^^^^                                  22450  800003
-------------------------------------------------------------------
 Illegal use of nuclide                   field  4
  REACTION   (68-ER-OXI(N,THS)68-ER-OXI,COH,AMP) Coherent Scattering
                              ^^^^^^^^^                                  22450  900003
-------------------------------------------------------------------

and similar messages for  ENTRY 22451.
                            REFERENCE  (J,ZN/A,52,270,1997)

==================================================

 To avoid error messages
  "Illegal code in                         field  1"

it is sufficient to add codes "67-HO-CMP" and "67-HO-OXI"  in Exfor
Dictionary 9 - Compounds.

 To avoid error message
 "Illegal use of nuclide                   field  4"

it would be necessary to add "3" to field 15 in Dict. 27. But this
latter doesn't contain compounds. On this reason this "3" has to be
added in corresponding fields of Daniel Dict.27.

=====================================================================
```

Stanislav Maev