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POSSIBLE AMENDMENTS TO THE NOMENCLATURE AND EXPLANATORY NOTES TO
CLARIFY THE CLASSIFICATION OF CO-ORDINATION COMPOUNDS

(Item II.3 on Agenda)

Reference documents :

40.212 (SSC/11)
40.460, Annex A/10 (SSC/11 - Report)
40.412 (HSC/18)
40.759 (SSC/12)
40.870, Annex A/13 (SSC/12 - Report)
41.100, Annex D/1, paragraph 22 (HSC/19 - Report)
41.663 (SSC/13)

I. BACKGROUND

Following the publication of Doc. 41.663, the Secretariat received, on 19 November 1997, a note from the Canadian Administration, which offers further proposals concerning the Explanatory Notes. The Canadian comments are excerpted below.

II. COMMENTS BY THE CANADIAN ADMINISTRATION

1. "As a result of the decision of the Scientific Subcommittee to modify Heading 29.42 to cover co-ordination compounds, we have drafted new Explanatory Notes for the heading. The changes will result in the shifting of some co-ordination compounds which are currently in other headings. We have tried to be as complete as possible in examining the possible ramifications of these changes and we are submitting a proposal for the consideration of the Scientific Subcommittee. We have included the rationale for the various changes we are proposing. Our comments on document 41.663 and our proposed Explanatory Notes are :
 - (a) We agree with the new text for heading 29.42, as proposed by the Secretariat.
 - (b) Because of the proposed addition of co-ordination compounds to heading 29.42, some compounds which are presently classified in other headings will now be classified in heading 29.42. Some co-ordination compounds which have been discussed previously

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by the Scientific Sub-Committee, for example those with alkyl radicals, carbonyl groups, unsaturated or aromatic hydrocarbons as ligands, would be moved to heading 29.42. Some of these compounds are mentioned in the EN, for example, iron and nickel carbonyls (heading 29.31). In our view, the new EN for heading 29.42 should specifically describe these types of compounds and the EN to headings 29.30 and 29.31 should specifically exclude them (see [proposals]).

- (c) The insertion of new item (1) on page 446 of the EN [see Annex, Doc. 41.663] for co-ordination compounds suggests that the renumbered items (2) to (7) are not co-ordination compounds. Some of these are co-ordination compounds and should be listed in item (1) (see [proposals]).
- (d) Many compounds of lower oxidation states of the transition metals are ionic. Some of the carboxylic acid "salts" of transition metals may be more ionic while others may be more covalent. Since it is not clear from the literature which compounds are salts and which are co-ordination compounds, we would prefer to refer to these compounds as "compounds of carboxylic acids with transition metals". We agree that it would be simpler to classify all of the compounds of carboxylic acids with transition metals in heading 29.42. It would be desirable to name the transition metals (which would not otherwise be excluded), as proposed by the Secretariat.

Similarly, we would also like to clarify the classification of transition metal alcoholates (alkoxides). According to chapter note 5(d) to chapter 29, metal alcoholates are to be classified in the same heading as their corresponding alcohols. With the introduction of a heading for co-ordination compounds, the classification of these compounds will be affected. Many alkoxides of transition metals are called "complexes" in the literature and should be considered co-ordination compounds. We propose that the Chapter notes be modified and that the EN to heading 29.42 include all alkoxides of transition metals.

- (e) We agree with the wording of the proposed new note which specifically includes metal fullerenes in heading 29.42. The inclusion of metal fullerenes in heading 29.42 is consistent with the classification of other organometallic compounds, such as metal carbonyls, in this heading.

2. In order to distinguish between the alcoholates (alkoxides) of elements such as sodium and potassium and the co-ordination compounds such as titanium tetra-*n*-butoxide, Chapter Note 5 (d) to Chapter 29 should be amended to read as follows :

“(d) Metal alcoholates of Group IA and IIA elements are to be classified in the same heading as the corresponding alcohols, except in the case of ethanol (heading No. 29.05).”.

III. SECRETARIAT COMMENTS

3. While the Canadian Administration agrees, in principle, with the proposals set out by the Secretariat in the Annex to Doc. 41.663, it also offers additional legal and Explanatory Note amendments which could provide more in-depth guidance concerning the classification of co-ordination compounds.
4. To simplify the discussion, the Secretariat has combined the proposals from Doc. 41.663 with the additional proposals made by Canada. The combined proposed legal amendments and the combined Explanatory Note amendments are set out in Annexes A and B, respectively, to this document. It is suggested, therefore, that these Annexes be used as the basis for discussion.
5. As noted by Canada in paragraph 2 above, it is proposed to amend Note 5 (d) to Chapter 29 to ensure that the Note applies only to alcoholates of non-transition metals, i.e., those falling in Groups IA and IIA of the IUPAC periodic table of elements. The transition metal alcoholates would fall to heading 29.42 by virtue of their co-ordinate or nearly co-ordinate bonding. A related amendment is also proposed by Canada for the exclusionary Explanatory Note to heading 29.20 (page 394). To simplify these proposed amendments, the Secretariat has referred to Group IA and IIA elements as “alkali metals or alkaline-earth metals”.
6. As for new Note 8 to Chapter 29, Canada suggests in paragraph 1 (d) above that “transition metal salts of [organic] [carboxylic] acids” would be more appropriately described as “compounds of carboxylic acids with transition metals”, since the ionic bonding which is usually associated with salts may not always be evident in transition metal salts. Therefore, both these options are presented in square brackets in the exclusionary text at the end of Part (A) of the proposed Explanatory Note amendments set out in Annex B.
7. In this connection, however, Canada also notes that it would be preferable to include all transition metal compounds in heading 29.42 (see also paragraph 7 of Doc. 41.663, in which the Secretariat suggested that it might be preferable to include all transition metal salts in heading 29.42). If this approach were to be pursued, proposals for amending Note 5 (d) and inserting new Note 8 to Chapter 29, as well as the proposed amendments to the Explanatory Notes to headings 29.20, 29.31 and 29.42, would need to be modified accordingly. The Sub-Committee is requested to give its views in this regard.
8. Given that co-ordination compounds generally involve a non-carbon (metal) element and an organic ligand, the Canadian Administration has also proposed amendments to the exclusionary Explanatory Note to heading 29.31 (covering organo-inorganic compounds) to clarify the fact that, despite their organo-inorganic nature, co-ordination compounds are classifiable in heading 29.42.
9. Finally, Canada has proposed a more elaborate description of the co-ordination compounds included heading 29.42 (see Part (A) of the proposed Explanatory Note to heading 29.42 in Annex B).

IV. CONCLUSION

10. The Sub-Committee is invited to examine the proposed legal and Explanatory Note amendments in Annexes A and B, respectively, taking into account the comments of the Canadian Administration in paragraphs 1 and 2 above, as well as those of the Secretariat in Doc. 41.663 and in paragraphs 3 to 9 above.
11. In particular, the Sub-Committee is requested to give its views concerning the possibility of including all transition metal compounds in heading 29.42 (see paragraph 7 above).

x

x x

(SCS/13/déc. 97)
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ANNEXE A

PROJET D'AMENDEMENT DE LA NOMENCLATURE CONCERNANT LES
COMPOSES DE COORDINATION

(Point II.3 de l'ordre du jour)

ANNEX A

POSSIBLE AMENDMENTS TO THE NOMENCLATURE CONCERNING
CO-ORDINATION COMPOUNDS

(Item II.3 on Agenda)

PROCEDURE DE L'ARTICLE 16

AMENDEMENT DE LA NOMENCLATURE

CHAPITRE 29

Note 5 d).

Nouvelle rédaction :

“d) Les alcoolates des métaux alcalins ou alcalino-terreux sont à classer dans la même position que les alcools correspondants sauf dans le cas de l'éthanol (n° 29.05).”.

Nouvelle Note 8.

Insérer la nouvelle Note de Chapitre suivante :

[Secrétariat :

“8.- Le n° 29.42 ne comprend pas les sels métalliques de transition des acides [organiques][carboxyliques] [qui contiennent un cation de titane, de vanadium, de chrome, de manganèse, de fer, de cobalt, de nickel, de cuivre, de zirconium, de niobium, de molybdène, de hafnium, de tantale, de tungstène ou de rhénium], même s'ils contiennent des liaisons de coordination.”.]

ou

[Canada :

“8.- Le n° 29.42 ne comprend pas les composés des acides carboxyliques avec des métaux de transition, [qui contiennent un cation de titane, de vanadium, de chrome, de manganèse, de fer, de cobalt, de nickel, de cuivre, de zirconium, de niobium, de molybdène, de hafnium, de tantale, de tungstène ou de rhénium], même s'ils contiennent des liaisons de coordination.”.]

N° 29.42.

Nouvelle rédaction :

“29.42 2942.00 Composés de coordination, (autres que les produits du n° 29.36); autres composés organiques.”.

x

x x

ARTICLE 16 PROCEDURE

AMENDMENTS TO THE NOMENCLATURE

CHAPTER 29

Note 5 (d).

Delete and substitute :

“(d) Alcoholates of alkali metals or alkaline-earth metals are to be classified in the same heading as the corresponding alcohols, except in the case of ethanol (heading No. 29.05).”.

New Note 8.

Insert the following new Chapter Note :

[Secretariat :

“8.- Heading No. 29.42 excludes transition metal salts of [organic][carboxylic] acids[, containing one of the cations titanium, vanadium, chromium, manganese, iron, cobalt, nickel, copper, zirconium, niobium, molybdenum, hafnium, tantalum, tungsten or rhenium], even if they contain co-ordinate bonds.”.]

or

[Canada :

“8.- Heading No. 29.42 excludes compounds of carboxylic acids with transition metals[, containing one of the cations titanium, vanadium, chromium, manganese, iron, cobalt, nickel, copper, zirconium, niobium, molybdenum, hafnium, tantalum, tungsten or rhenium], even if they contain co-ordinate bonds.”.]

Heading 29.42

Delete and substitute :

“**29.42** 2942.00 **Co-ordination compounds (excluding products of heading No. 29.36); other organic compounds.**”.

x

x x

ANNEXE B

PROJET DE MODIFICATION DES NOTES EXPLICATIVES CONCERNANT LES
COMPOSES DE COORDINATION

(Point II.3 de l'ordre du jour)_

ANNEX B

POSSIBLE AMENDMENTS TO THE EXPLANATORY NOTES CONCERNING
CO-ORDINATION COMPOUNDS

(Item II.3 on Agenda)_

PROCEDURE DE L'ARTICLE 16
MODIFICATION DES NOTES EXPLICATIVES

CHAPITRE 29.

Page 342.

1. Note 5 d).

Nouvelle rédaction :

“d) Les alcoolates des métaux alcalins ou alcalino-terreux sont à classer dans la même position que les alcools correspondants sauf dans le cas de l'éthanol (n° 29.05).”.

2. Nouvelle Note 8.

Insérer la nouvelle Note de Chapitre suivante :

[Secrétariat :

“8.- Le n° 29.42 ne comprend pas les sels métalliques de transition des acides [organiques][carboxyliques] [qui contiennent un cation de titane, de vanadium, de chrome, de manganèse, de fer, de cobalt, de nickel, de cuivre, de zirconium, de niobium, de molybdène, de hafnium, de tantale, de tungstène ou de rhénium], même s'ils contiennent des liaisons de coordination.”.]

ou

[Canada :

“8.- Le n° 29.42 ne comprend pas les composés des acides carboxyliques avec des métaux de transition, [qui contiennent un cation de titane, de vanadium, de chrome, de manganèse, de fer, de cobalt, de nickel, de cuivre, de zirconium, de niobium, de molybdène, de hafnium, de tantale, de tungstène ou de rhénium], même s'ils contiennent des liaisons de coordination.”.]

Page 394. N° 29.20. Dernier paragraphe (exclusion).

Nouvelle rédaction :

“La présente position **ne couvre pas** :

- a) les alcoolates (alkoxydes) de métaux alcalins ou alcalino-terreux, classés avec les alcools auxquels ils correspondent (voir la Note 5 d) du présent Chapitre).
- b) les composés de coordination, y compris les alkoxydes de métaux de transition, comme par exemple le tétra-*n*-butoxyde de titane, dénommé également titanate de tétrabutyle (n° 29.42).”

ARTICLE 16 PROCEDURE

AMENDMENTS TO THE EXPLANATORY NOTES

CHAPTER 29

Page. 342.

1. Note 5 (d).

Delete and substitute :

- (d) Alcoholates of alkali metals or alkaline-earth metals are to be classified in the same heading as the corresponding alcohols, except in the case of ethanol (heading No. 29.05).

2. New Note 8.

Insert the following new Chapter Note 8 :

[Secretariat :

“8. - Heading No. 29.42 excludes transition metal salts of [organic][carboxylic] acids[, containing one of the cations titanium, vanadium, chromium, manganese, iron, cobalt, nickel, copper, zirconium, niobium, molybdenum, hafnium, tantalum, tungsten or rhenium], even if they contain co-ordinate bonds.”.]

or

[Canada :

“8. - Heading No. 29.42 excludes compounds of carboxylic acids with transition metals[, containing one of the cations titanium, vanadium, chromium, manganese, iron, cobalt, nickel, copper, zirconium, niobium, molybdenum, hafnium, tantalum, tungsten or rhenium], even if they contain co-ordinate bonds.”.]

Page 394. Heading 29.20. Last paragraph (exclusion).

Delete and substitute :

“This heading **excludes** :

- (a) Alcoholates (alkoxides) of alkali metals or alkaline-earth metals, which are classified with their respective alcohols (see Note 5 (d) to this Chapter).
- (b) Co-ordination compounds, including transition metal alkoxides, e.g., titanium tetra-*n*-butoxide (also known as tetrabutyl titanate) (**heading 29.42**).”

Page 412. N° 29.31. Dernier paragraphe (exclusion).

Nouvelle rédaction :

“La présente position **ne comprend pas** :

- a) les thiocomposés organiques dont la molécule comporte un ou plusieurs atomes de soufre directement liés à l'atome (aux atomes) de carbone (voir la Note 6 du présent Chapitre). Sont exclus les composés dont la molécule comporte, outre des atomes de soufre directement liés à l'atome (aux atomes de carbone), d'autres éléments non métalliques ou métalliques directement liés à l'atome (aux atomes) de carbone (par exemple, le fonofos (ISO)) (n° 29.30).
- b) les alkyles de métaux de transition, les fullerènes métalliques et les composés complexes de métaux (y compris les métallocènes et les métaux carbonyles, comme par exemple le ferrocène et le fer carbonyle) (n° 29.42).”

Page 446. N° 29.42.

Nouvelle rédaction :

“29.42 - COMPOSES DE COORDINATION (AUTRES QUE LES PRODUITS DU N° 29.36); AUTRES COMPOSES ORGANIQUES.”.

A- COMPOSES DE COORDINATION

Les composés de coordination (complexes) contiennent un ion central (d'ordinaire un métal de transition) et un ou plusieurs ligands organiques qui, ensemble, forment un complexe dont les liaisons ne sont ni covalentes ni ioniques mais intermédiaires entre ces deux types. Le complexe peut être cationique, anionique ou nonionique suivant la somme des charges de l'atome central et du ou des ligands. Sont inclus dans la présente position sont les composés en cage, y compris les complexes internes et externes de fullerène.

Les composés de coordination couverts par la présente position couvrent notamment :

- 1) **Les composés complexes contenant de simples ligands donneurs** : le ligand partage une ou plusieurs paires d'électrons avec l'atome de métal. Les ligands peuvent comporter une seule liaison ou plusieurs liaisons. Un ligand comportant une seule liaison est relié au métal par un seul de ses atomes. Un ligand comportant plusieurs liaisons est relié au métal par plusieurs de ses atomes (composés complexes d'éthylènediamine, par exemple). Les composés de coordination dont les ligands comportent plusieurs liaisons sont appelés chélates.

La présente partie comprend notamment :

- a) **les composés complexes d'éthylènediamine**
- b) **les composés complexes de chélatés dicétonate**
- c) **les alkoxydes de métaux de transition**
- d) **les composés complexes** du fluorure de bore avec l'acide acétique, l'éthylrique éther ou le phénol
- e) **l'acéto-arsénite de cuivre** (*vert de Schweinfurt*)
- f) **les gluconates antimonio-sodiques** (antimoine tri- ou pentavalent).

- 2) **Les composés complexes métalliques** : composés dans lesquels les électrons du ligand (des ligands) participent à la liaison. Le ligand donne des électrons au métal, mais comporte également des orbitales d'accueil qui peuvent accepter des électrons du métal (back-bonding). Comme ces ligands peuvent accepter des électrons, ils sont appelés ligands acides. Les molécules et ions organiques qui peuvent former des composés complexes métalliques comprennent notamment l'oxyde de carbone, les oléfines, les ions cyclopentadiényles (métallocènes) et les ions tropylium.

La présente partie couvre notamment :

- a) le ferrocène
- b) le fer carbonyle et autres métaux carbonyles

- 3) **Autres composés organométalliques** : autres composés à liaisons carbone - métal

La présente partie comprend notamment :

- a) les alkyles de métaux de transition
- b) les fullerènes métalliques

B.- AUTRES COMPOSES ORGANIQUES

La présente partie couvre les composés organiques de constitution chimique définie présentés isolément qui ne peuvent être classés ailleurs.

- 1) **Cétènes**. Comme les cétones, ils se caractérisent par un groupement carbonyle ($>C=O$). Toutefois, dans les cétones, le groupement carbonyle est lié à l'atome de carbone voisin par une double liaison (cétène, diphénylcétène, par exemple).

La présente position **exclut** toutefois le dicétène qui est une lactone du **n° 29.32**.

- 2) **Di-iodure de dithymol**.
- 3) **Méthacrylochlorure de chrome**.

Toutefois, la présente position **ne comprend pas** les produits compris par la Note 1 de Section VI ou d'autres composés de coordination tels que la vitamine B₁₂ et ses dérivés (**n° 29.36**) [ou les [sels] [composés] métalliques de transition des acides [organiques] [carboxyliques] [composés des acides carboxyliques avec des métaux de transition] [qui contiennent un cation de titane, de vanadium, de chrome, de manganèse, de fer, de cobalt, de nickel, de cuivre, de zirconium, de niobium, de molybdène, de hafnium, de tantale, de tungstène ou de rhénium] (voir la Note 8 du présent Chapitre).”

Page 412. Heading 29.31. Last paragraph (exclusion).

Delete and substitute :

“This heading **excludes** :

- (a) Organo-sulphur compounds whose molecules have sulphur atom(s) directly linked to carbon atom(s) (see Note 6 to this Chapter). It excludes compounds whose molecules contain, in addition to sulphur atom(s) directly linked to carbon atom(s), other non-metal or metal atom(s) directly linked to carbon atom(s) (e.g., fonofos (ISO)) (**heading 29.30**).
- (b) Transition metal alkyls, metal fullerenes and metal complexes (including metallocenes and metal carbonyls, e.g., ferrocene, iron carbonyl) (**heading 29.42**).”

Page 446. Heading 29.42.

Delete and substitute :

“29.42 - CO-ORDINATION COMPOUNDS (EXCLUDING PRODUCTS OF HEADING No. 29.36); OTHER ORGANIC COMPOUNDS.”

(A) CO-ORDINATION COMPOUNDS

Co-ordination (complex) compounds comprise a central atom or ion (usually a transition metal) and one or more organic ligands, which together form a complex with bonding that is neither covalent nor ionic, but intermediate between the two types. The complex may be cationic, anionic or non-ionic, depending on the sum of the charges of the central atom and the ligand. The heading also includes polytopal (cage) compounds, such as internal and external fullerene complexes.

The co-ordination compounds covered by this heading include :

- (1) **Complexes with simple donor ligands** : the ligand shares one or more electron pairs with the metal atom. Ligands can be unidentate or multidentate. A unidentate ligand is connected to the metal through only one of its atoms. A multidentate ligand is connected to the metal through more than one of its atoms (e.g., ethylenediamine complexes). Co-ordination compounds with multidentate ligands are known as chelates.

This part includes, *inter alia*:

- (a) **Ethylenediamine complexes.**
- (b) **Diketonate chelate complexes.**
- (c) **Alkoxides of transition metals.**
- (d) **Boron trifluoride complexes** with acetic acid, dimethyl ether or phenol.
- (e) **Copper acetoarsenite** (Schweinfurt green).
- (f) **Sodium antimonylgluconate** and **sodium stibogluconate** (tri- or pentavalent antimony).

- (2) **Metal complexes** : complexes in which the electron system of the ligand(s) is involved in bonding. The ligand donates electrons to the metal but also has acceptor orbitals which can accept electrons from the metal (back-bonding). Because these ligands can accept electrons, they are called acid ligands. Organic molecules and ions which can form metal complexes include carbon monoxide, olefins, cyclopentadienyl ions (metallocenes), tropylium ions, etc.

This part includes, *inter alia* :

- (a) **Ferrocene.**
(b) **Iron carbonyl and nickel carbonyl.**
- (3) **Other organometallic compounds** : other compounds with carbon-metal bonds.

This part includes, *inter alia* :

- (a) **Transition metal alkyls.**
(b) **Metal fullerenes.**

(B) OTHER ORGANIC COMPOUNDS

This part covers separate chemically defined organic compounds not classified elsewhere.

- (1) **Ketenes.** Like ketones, these are characterised by a carbonyl group ($>C=O$). However, in ketenes, the carbonyl group is linked to the neighbouring carbon atom by a double bond (e.g., ketene, diphenylketene).

This heading however **excludes** diketene which is a lactone of **heading 29.32**.

- (2) **Dithymol di-iodide.**
(3) **Methacrylate chromic chloride .**

However, this heading **does not include** products covered by Note 1 to Section VI or other co-ordination compounds of **heading 29.36**, such as vitamin B₁₂ and its derivatives, [or transition metal salts of [organic] [carboxylic] acids] [compounds of carboxylic acids with transition metals] [, containing one of the cations titanium, vanadium, chromium, manganese, iron, cobalt, nickel, copper, zirconium, niobium, molybdenum, hafnium, tantalum, tungsten or rhenium] (see Note 8 to this Chapter).".