

# WIPO



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**WORLD INTELLECTUAL PROPERTY ORGANIZATION**  
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**SPECIAL UNION FOR THE INTERNATIONAL PATENT CLASSIFICATION  
(IPC UNION)**

**IPC REVISION WORKING GROUP**

**Seventh Session  
Geneva, June 10 to 21, 2002**

**INTRODUCTION OF ILLUSTRATING CHEMICAL FORMULAE IN THE  
ELECTRONIC LAYER OF THE IPC**

*Document prepared by the Secretariat*

1. At its fifth session, held in June 2001, the IPC Revision Working Group asked volunteering offices to comment on the chemical formulae provided by the Korean Intellectual Property Office. Comments were submitted on the formulae of all IPC areas indicated in Annex H to document IPC/WG/6/5, with the exception of subclass C 09 B. These comments are available on the IBIS Web site ([www.wipo.int/ibis/temp/chem-2002-jun/index.htm](http://www.wipo.int/ibis/temp/chem-2002-jun/index.htm)).
2. The Annex to this document contains a paper submitted by Germany with "Questions and Remarks Concerning the Chemical Formulae Project." It is proposed that this paper serve as the basis for the discussion of the procedure to be adopted for the continuation of this project.

[Annex follows]

**E**

ANNEX

To: "mikhail.makarov@wipo.int" <mikhail.makarov@wipo.int>  
Subject: chemical formulae project  
From: IPC-DE <IPC-DE@dpma.de>  
Date: Wed, 10 Apr 2002 12:25:20 +0200  
Cc: Okelmann Axel <Axel.Okelmann@dpma.de>

Dear Mr. Makarov,

We have some questions and remarks concerning the chemical formulae project:

- 1) Now that most of the contributions for this project have been distributed, it has become apparent that the format and style of the drawings should have been fixed beforehand. It is not clear to us whether all offices have used the .skc format, since in some documents the formulae are not embedded as .skc files but as graphical images, and thus cannot be opened with a chemical drawing program. Also, the settings for the style should have been fixed, e.g. line thickness, font of atom symbols, bond length (and also the angles of the bonds should be used according to the default settings cf. A61K31/7032 from EP).
- 2) There is also an inconsistency concerning the use of formulae for concrete compounds and general formulae. In our opinion, general formulae should be used in main groups and subgroups that are higher in the hierarchy. To make the difference clear to the user, these formulae could e.g. be printed in bold and have the addition of "general formula". In all other subgroups, formulae for concrete compounds, to be classified in a given group, could be used and, to make obvious that this is only one possible example, could be added "e.g."
- 3) In cases where the title lists several classes of compounds (e.g. C07D 211/34 ..... with hydrocarbon radicals, substituted by carbon atoms having three bonds to hetero atoms with at the most one bond to halogen, e.g. ester or nitrile radicals) or several concrete compounds (e.g. C12P 13/06 . . Alanine; Leucine; Isoleucine; Serine; Homoserine) the number of formulae to be used for illustration should be agreed upon. We would prefer only one compound in each group (perhaps with the name attached to the formula when required for clarity).

- 4) In some entries, examples of high complexity were chosen for illustration; we would prefer to use compounds that are as simple as possible.
- 5) In our opinion, the use of 3-dimensional formulae (e.g. for carbohydrates) and 2-dimensional formulae should be fixed; especially mixing should be avoided (cf. A61K31/7032 from EP). We would prefer to use only 2D formulae except when it is absolutely necessary to use 3D).
- 6) Different conventions have been used for substituents such as methyl (“-” or “-CH3”); this should also be harmonised (other cases are e.g. -COOH, -C6H5, -Et, -CN, N3, NO2).
- 7) In cases where the compounds mentioned in the title are only used but not prepared (e.g. C12P 19/18 . produced by the action of a glycosyl transferase, e.g. alpha-, beta- or gamma-cyclodextrins) we would prefer not to include any formulae.
- 8) Sometimes, formulae with numbering have been used (cf. A61K31/518 EP). It should be agreed upon whether this is appropriate and, if so, in which specific cases. We would prefer not to use numbering (or only in general formulae).
- 9) In our opinion a procedure for a rapporteur/commentary system should be installed. Perhaps there should be, in addition to the original commenting office, one other office designated for comment (of course, all other offices would be able to comment too, but to check all areas would be too time-consuming). This designated office would have to check not only the corrected formulae but also the original KIPO proposal.

Best regards,  
Klaus Vogt  
German Patent and Trade Mark Office

[End of Annex and of document]