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D E C I S I O N
of 13 January 2006

Case Number: T 0654/02 - 3.3.01

Application Number: 96909711.2

Publication Number: 0764168

IPC: C07D 487/22

Language of the proceedings: EN

Title of invention:

Heteroatom-functionalized porphyrazines and multimetallic complexes and polymers derived therefrom

Applicant:

Hoffman/BARRETT, L.L.C

Opponent:

-

Headword:

Porphyrazines/HOFFMAN-BARRETT

Relevant legal provisions:

EPC Art. 123(2), 84, 83, 54, 56, 111(1)

Keyword:

"Amendments allowable (yes) - directly and unambiguously disclosed"

"Clarity of functional features (yes)"

"Sufficiency of disclosure (yes)"

"Novelty (yes)"

"Inventive step (yes) - non obvious solution"

"Remittal for further prosecution (yes)"

Decisions cited:

-

Catchword:

-



Case Number: T 0654/02 - 3.3.01

D E C I S I O N
of the Technical Board of Appeal 3.3.01
of 13 January 2006

Appellant:

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Decision under appeal:

Decision of the Examining Division of the
European Patent Office posted 17 December 2001
refusing European application No. 96909711.2
pursuant to Article 97(1) EPC.

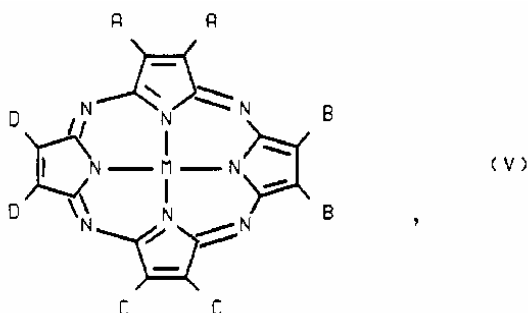
Composition of the Board:

Chairman: A. Nuss
Members: P. Ranguis
R. Menapace

Summary of Facts and Submissions

- I. The present appeal lies from the decision of the Examining Division to refuse the European patent application No. 96 909 711.2 (European publication No. 764 168) pursuant to Article 97(1) EPC.
- II. The decision under appeal was based on a set of thirty seven claims filed before the Examining Division with a letter received on 2 November 2000. Claim 1 read as follows:

"1. A heteroatom-functionalized porphyrazine compound having the structure:



wherein M is 2H or an element capable of complexing with pyrrole nitrogen atoms, and A, B, C and D are independently selected from the group consisting of a thio moiety, an amino moiety, an oxo moiety, a phospho moiety, a seleno moiety, a telluro moiety and a hydrocarbon moiety, wherein at least two of A, B, C and D are capable of complexing with a metal ion M^1 and wherein the porphyrazine compound V is capable of complexing two or three metal ions M^1 to its periphery."

III. The Examining Division acknowledged novelty of the subject-matter of Claim 1. However, it found that the subject-matter of Claim 1 of this request lacked inventive step over documents

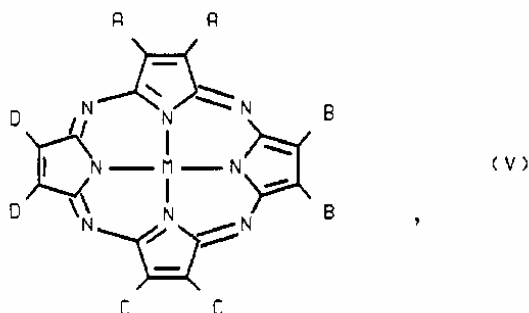
(1) J. Am. Chem. Soc. **1994**, 116, 2639-2640 and

(3) J. Chem. Soc., Chem. Commun., **1994**, 2095-2096

Document (1) which related to porphyrazines containing one peripheral complexed metal ion and document (3) which related to porphyrazines containing four peripheral complexed metal ions provided incentive for preparing further multi-metallic porphyrazines. Furthermore, the application as originally filed presented mono-, bi-, tri- and tetra-metallic complexes as having equivalent properties. In the absence of any unexpected properties related to the compounds falling within the claimed area with respect to the compounds disclosed in document (1) and (3), the claimed subject-matter of Claim 1 did not involve an inventive step.

IV. At the oral proceedings before the Board which took place on 13 January 2006, the Appellant filed as sole request a set of twenty seven claims. Claim 1 reads as follows:

"1. A heteroatom-functionalized porphyrazine compound having the structure:



wherein M is 2H or an element capable of complexing with pyrrole nitrogen atoms, and A, B, C and D are independently selected from the group consisting of a thio moiety selected from the group consisting of sulfo; sulfhydryl; alkylthio (-SR), wherein R is an alkyl group having one to 10 carbon atoms, a polyethylene oxide chain having one to twenty ethylene oxide units, phenyl, benzyl or allyl, or R is a benzyl blocking group; -SSi(R₇)₃, wherein the R₇ groups are independently selected from an alkyl group having one to 16 carbon atoms and phenyl; -SCH₂(CH₂)_cO(CH₂(CH₂)_cO)_dR₉ or -SCH₂(CH₂)_cS(CH₂(CH₂)_cO)_dR₉, wherein c is one or two, d is an integer from one to five, and R₉ is hydrogen or an alkyl group having one to 16 carbon atoms; and -SCH₂(CH₂)_cE(CH₂(CH₂)_cF)_dR₉, wherein E and F are independently selected from the group consisting of selenium, tellurium, alkylamino wherein the alkyl group has one to 16 carbon atoms, alkyl wherein the alkyl group has two to ten carbon atoms, p-toluenesulfonamide, 2-pyridylmethyl, COCH₂COR₉, CH₂COCH₂COR₉, CH₂CO₂H, and acetamide, and a hydrocarbon moiety, wherein two or three of A, B, C and D are capable of complexing with a metal ion M¹ and wherein the porphyrazine compound V is capable of complexing two or three metal ions M¹ to its periphery."

V. The Appellant argued that the Examining Divisions' assessment regarding inventive step had been reached with the benefit of hindsight since neither document (1) nor document (3) suggested compounds capable of complexing two or three metal ions M^1 to its periphery.

Document (1) described compounds comprising only one peripheral complexed metal ion. Although those compounds were soluble, they could not be polymerised.

Contrary to the Examining Divisions' finding, the indication that the binucleating ligand system permitted the preparation of a wide variety of metal complexes whose novel spectroscopic and magnetic properties would be the subject of future reports did not address the possibility of changing the numbers of peripheral metal ions but was related to the possibility of changing the type of the metal ions complexed by the nucleating agent.

Document (3) taught only pentametallic porphyrzine complexes. None of the moieties could be selected to improve the solubility of the complexes.

The claimed compounds exhibited spectroscopic and magnetic properties which could be better adjusted with three or four metal ions rather with only two metal ions as suggested in document (1). Furthermore, the multi-metallic compounds according to Claim 1 could be linked to provide oligomers and polymers by edge-sharing the metal ions complexed at their periphery. Document (3) was silent with regard to these opportunities and the solitaire porphyrzines of document (1) were not able to form polymers. It was

furthermore pointed out that the claimed compounds exhibited a combination of optical, chemical and biological properties which rendered them valuable as imaging agents.

- VI. The Appellant requested that the decision under appeal be set aside and that a patent be granted on the basis of the set of claims 1 to 27 as submitted during the oral proceedings.
- VII. At the end of the oral proceedings the decision of the Board was announced.

Reasons for the Decision

1. The appeal is admissible.
2. *Amendments*
 - 2.1 The porphyrazine compounds (V) according to Claim 1 represent a restriction compared to the general definition disclosed in the application as originally filed.

From the description, it derives that the moieties A, B, C and D that are capable of complexing with a metal ion M^1 are sulfo, oxo, amino, phospho, seleno or telluro moieties (see page 5, lines 5 to 7 and page 16, lines 11 to 13), whereas the hydrocarbon moiety is a noncoordinating moiety (see page 5, lines 7-8 and page 13, lines 2-3). Therefore, limiting the claimed subject-matter to a thio as moiety capable of complexing with a metal ion M^1 is directly and

unambiguously derivable from the content of the application as originally filed.

From the description it can also be derived directly and unambiguously that the porphyrazine compounds (V) can comprise two or three of A, B, C and D capable of complexing with a metal ion M^1 and said compounds are capable of complexing two or three metal ions M^1 to their periphery (see formulas (VII), (VIII) and (IX), page 14).

The specific definition of the thio moiety finds support on page 18, line 32 to page 19, line 25 of the application as filed.

- 2.2 From the above, it is concluded that the subject-matter of Claim 1 does not extend beyond the content of the application as originally filed in compliance with the requirement of Article 123(2) EPC.

3. *Clarity*

The functional features "wherein two or three of A, B, C and D are capable of complexing with a metal ion M^1 and wherein the porphyrazine compound V is capable of complexing two or three metal ions M^1 to its periphery" are directly related to the structurally defined thio moiety. For this reason, there is no objection against the subject-matter of Claim 1 under Article 84 EPC.

4. *Sufficiency of disclosure*

In view of the description, the Board is satisfied that the subject-matter of Claim 1 is disclosed in a manner

sufficiently clear and complete for it to be carried out by a person skilled in the art (see page 18, lines 5 to 12; page 36, line 3 to page 37, line 22 and page 52, lines 3 to 11). The requirement of Article 83 EPC is hence met as far as Claim 1 is concerned.

5. *Novelty*

After examining of the cited prior art documents, the Board has reached the conclusion that the subject-matter of Claim 1 is novel. Since novelty of Claim 1 of the request before the Examining Division was not contested (cf. point III above) and since the subject-matter of Claim 1 of the present request represents a restriction vis-à-vis Claim 1 of the request before the Examining Division (cf. points II and IV), it is not necessary to give detailed reason for the finding.

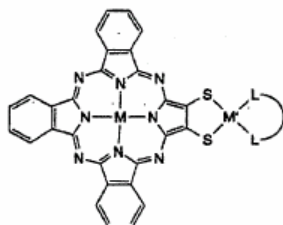
6. *Inventive step*

- 6.1 The subject-matter of Claim 1 relates to heteroatom-functionalized porphyrzine compounds of formula (V) capable of complexing two or three metal ions M^1 to their periphery (cf. point IV above).

The claimed porphyrzine compounds have applications as magnetic materials, molecular metal conductors, imaging agents and dyes (see page 1, lines 27 to 31 and page 11, lines 18 to 20). Such porphyrzine compounds are also used to prepare multimetallic porphyrzine compounds, porphyrzines-based oligomers and polymers with similar properties and applications (see page 1, lines 24 to 31, page 6, lines 3 to 5, page 9, lines 2 to 10; page 12, lines 13 to 19; page 18, lines 19 to 23; page 32,

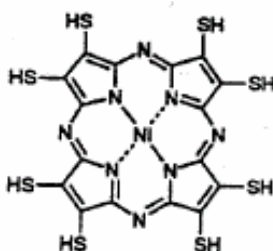
lines 8 to 11, page 52, lines 3 to 11 and page 59, lines 13 to 31).

- 6.2 Document (1) discloses solitaire porphyrazines of the formula:



obtained through capping the corresponding norphthalocyanine dithiolates with (P-P)PdCl₂, wherein M is 2H, Ni or Cu, M' is Pd and the ligand couple L-L is a bisdiphenylphosphine ferrocene (see page 2639, right-hand column). The optical spectra of the precursors along with the solitaire porphyrazines were furthermore obtained (cf. Figure 2).

- 6.3 Document (3) discloses a porphyrazine octathiolate derivative of the formula:



and complexes isolated with four metal cations peripherally bonded to the eight thiolate residues via quadruple bidentate or tridentate coordination to provide a pentametallic porphyrazine. The porphyrazine octathiolate derivative is, therefore, a precursor of multimetallic porphyrazine compounds. Since due to their conjugated π -system, porphyrins and porphyrin derivatives are deeply colored and show characteristic

electronic-absorption spectra which vary with the chromophoric system and with the various substituents attached to the chromophore, it is clear to a skilled person that the specific porphyrin disclosed in document (3) also exhibits optical properties.

6.4 Since the claimed heteroatom-functionalized porphyrazine compounds are capable of complexing with two or three metal ions M^1 at their periphery, document (1) would be, from a structural point of view, the closest state of the art as far as the compounds capable of complexing two metal ions M^1 at their periphery are concerned. By contrast, document (3) would be the closest state of the art for the compounds capable of complexing three metal ions M^1 at their periphery. However, in accordance with the established jurisprudence the problem solution approach requires that the technical problem to be solved be defined with respect to one document as the starting point. The Board considers, therefore, in agreement with the Appellant document (3) the closest one on the ground that the claimed compounds are capable of complexing more than one metal ions M^1 at their periphery and, as a result, can form polymacrocyclic compounds, like the compound of document (3).

6.5 In view of document (3), the least ambitious technical problem to be solved can be seen in the provision of porphyrazines having spectroscopic properties for the use as imaging agents and dyes, and being useful as precursors of porphyrazines having metal ions at their periphery with similar properties and applications.

- 6.6 As a solution to the so defined technical problem, the present application proposes the heteroatom-functionalized porphyrazine compounds according to Claim 1.
- 6.7 In view of the description, the Board is satisfied that the technical problem is solved within the whole claimed area because it is credible, from a chemical point of view, that the claimed compounds have spectroscopic properties rendering them useful as imaging agents and dyes (see page 11, lines 18 to 23). In addition, they are precursors of multimetallic porphyrazines with similar properties and applications. Indeed, due to their unshared electron pair, thio moieties can complete with the help of ligands the coordination sphere of the peripherally complexed metal ions M^1 (see page 1, lines 27 to 31 and page 5, line 1 to page 6, line 1).
- 6.8 It remains to be decided whether or not the claimed solution to the technical problem defined above was obvious in view of the prior art cited. The question arises, in particular, which structural modifications to the disclosed compounds the person skilled in the art would have been encouraged to achieve in view of the whole teaching of documents (1) and (3).
- 6.8.1 The Examining Division was of the opinion that documents (1) and (3) both provided an incentive for the preparation of further multimetallic porphyrazines.
- 6.8.2 Document (3) discloses a complex with four metal cations peripherally bonded to the eight thiolate residues (cf. point 6.3 above). The teaching of

document (3) that these pentametallic porphyrzine complexes, denoted star porphyrzines, are of considerable interest for the study of indirect metal-metal interactions via porphyrzines π -system, alone does not constitute a pointer for the skilled person towards the claimed porphyrzines when trying to solve the technical problem as defined above. Indeed, said teaching rather directs the skilled person to other pentametallic complexes, as it is shown by the fact that the authors of document (3) actually propose as a follow up action to design pentametallic complexes of the porphyrzinoctamine type (see page 2095, scheme 3 and page 2096, right-hand column, first paragraph).

- 6.8.3 Document (1) discloses solitaire porphyrzines, namely porphyrzines complexed with one metal at their periphery through a couple of thio moieties (cf. point 6.2 above). As pointed out by the Examining Division, document (1) states that the binucleating ligand system permits the preparation of a wide variety of metal complexes whose novel spectroscopic and magnetic properties will be the subject of future reports. However, such a statement cannot be regarded as a pointer towards the claimed compounds, rather it directs the skilled person to change the metals of the complexes. Even when combining the teachings of document (1) and document (3), the skilled person would have been guided only to replace the peripheral thio moieties of the solitaire porphyrzines by amino moieties (cf. point 6.8.2 above) yielding other solitaire porphyrzines, but not to design porphyrzines capable of complexing two or three metal ions to their periphery.

6.8.4 Hence, in the absence of a prior art teaching in the relevant technical field a correlation between compounds capable of complexing two or three metal ions to their periphery and compounds capable of complexing one or four metal ions at their periphery, the skilled person when trying to solve the technical problem as defined above has no guidance towards the claimed compounds with the sole knowledge of documents (1) and (3). This is the point where the Board differs from the Examining Division which, in the Board's judgment, failed to substantiate the alleged obvious relationship between various polymetallic complexes. Such a relationship cannot be established *a posteriori*, namely with the knowledge of the application as originally filed containing in that respect considerations which represent neither common general knowledge nor knowledge derivable from any prior art.

6.8.5 In view of the above, the claimed subject-matter according to Claim 1, does not derive in an obvious manner from the prior art cited and for that reason involves an inventive step (Article 56 EPC).

7. *Remittal to the first instance - Article 111(1) EPC*

7.1 The Board has come to the conclusion that the subject-matter of Claim 1 complied with the requirements of the EPC overcoming, therefore, the reasons of refusal of the first instance. Having so decided, the Board has nevertheless not taken a decision on the case as a whole since the set of claims of the present request comprises other independent product claims related to multimetallic complexes, oligomers and polymers derived therefrom, the allowability of which must be examined

on their own merits. This examination is incumbent on the Examining Division in order not to deprive the Appellant of the possibility of being heard by the two instances provided, in respect of the matter at hand.

- 7.2 Under these circumstances, the Board finds it appropriate to exercise the power conferred on it by Article 111(1) EPC to remit the case to the department of first instance for further prosecution.

Order

For these reasons it is decided that:

1. The decision under appeal is set aside.
2. The case is remitted to the department of first instance for further prosecution on the basis of the claims 1 to 27 submitted at the oral proceedings before the Board.

The Registrar:

The Chairman:

N. Maslin

A. Nuss