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**D E C I S I O N**  
**of 17 March 1998**

**Case Number:** T 0578/96 - 3.4.2

**Application Number:** 90911386.2

**Publication Number:** 0489748

**IPC:** G01N 21/35

**Language of the proceedings:** EN

**Title of invention:**  
Improved octane measuring process

**Patentee:**  
Ashland Oil, Inc.

**Opponent:**  
BP Chemical S.N.C. Tour Neptune  
Bran + Luebbe GmbH

**Headword:**  
-

**Relevant legal provisions:**  
EPC Art. 54, 56

**Keyword:**  
"Novelty and inventive step (yes)"

**Decisions cited:**  
-

**Catchword:**  
-



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Boards of Appeal

Chambres de recours

Case Number: T 0578/96 - 3.4.2

**D E C I S I O N**  
of the Technical Board of Appeal 3.4.2  
of 17 March 1998

**Appellant:**  
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**Decision under appeal:** Decision of the Opposition Division of the  
European Patent Office posted 3 June 1996  
revoking European patent No. 0 489 748 pursuant  
to Article 102(1) EPC.

**Composition of the Board:**

**Chairman:** E. Turrini  
**Members:** R. Zottmann  
M. Lewenton

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## Summary of Facts and Submissions

- I. The Appellant (Patentee) lodged an appeal against the decision of the Opposition Division revoking the patent No. 0 489 748 with the application No. 90 911 386.2.

The oppositions were based on the grounds of Article 100(a) that the subject-matter of the patent lacked novelty and inventive step (Articles 52(1), 54 and 56 EPC) and on the grounds of Articles 100(b) and 100(c) EPC.

The Opposition Division held that the ground of opposition laid down in Article 100(b) did not prejudice the maintenance of the patent, did not maintain its objection with respect to Article 100(c) after an amendment and argued that claim 1 as granted (main request) was not novel with respect to document

E3: Anal. Chem. 1989, 61, pages 313 to 320  
("Prediction of Gasoline Octane Numbers from Near-Infrared Spectral Features in the Range 660-1215 nm"),

in substance since the t-butyl/methylene band (more specifically the third overtone) is used also in the measurements described in said document.

- II. The following further documents are cited in this (appeal) decision:

E7: Chemical Reviews 1959, pages 628 to 659 (Wheeler: "Near infrared spectra of organic compounds");

E10: B. G. Osborne et al.: "Near infrared spectroscopy food analysis", J. Wiley & Sons, 1986, pages 28 to 41;

- E12: "Römpps Chemie-Lexikon", 8<sup>th</sup> edition, Stuttgart, 1985, page 2576;
- E13: "Hackh's Chemical Dictionary", McGraw-Hill, 1969, pages 424 to 425;
- E15: "Nomenclature of organic chemistry", Pergamon Press, 1979, page 14;
- E16: "The vocabulary of organic chemistry", J. Wiley & Sons, 1980, pages 48 and 50;
- E17: H. Günzler; H. Böck: "IR-Spektroskopie: eine Einführung", Verlag Chemie, 1975, pages 154 to 159 and 359.

- III. In a letter of response, the Respondent II (Opponent II) commented on the arguments of the statement of the grounds of appeal. Respondent I (Opponent I) did not put forward any arguments during the appeal proceedings.
- IV. Later on both Opponents withdrew their oppositions.
- V. The Appellant requested that the decision under appeal be set aside and, as main request, that the patent be maintained as granted with decision of 29 July 1993, that is **without** the amendment according to the ERRATUM issued and published on 22 December 1993, having the consequence that the text of the patent specification at the end of line 21 of page 6 reads: "from about 1195-120". Subsidiarily, he requested that the patent be maintained on the basis of sets of amended claims, as auxiliary requests. He further requested that oral proceedings be held unless the Board accepts the appeal on the basis of the written record.

VI. Claim 1 of the main request (as granted) reads:

"1. A process for the measurement of octane number; or other measure of knock avoidance, of fuels by near infrared range spectroscopy, comprising determining said octane number or other measure of knock avoidance by:

- a. measuring infrared absorbance of the fuel in the t-butyl/methyne band;
- b. periodically or continuously outputting a signal indicative of the intensity of said absorbance in said band or one mathematical function or a combination of mathematical functions thereof; and
- c. mathematically converting said signal to an output signal indicative of said octane number or other measure of knock avoidance of said fuel."

Claims 2 to 9 are dependent on claim 1.

VII. The arguing of the Appellant with respect to the main request is summarized as follows:

It is clear that the skilled reader of the patent-in-suit would understand the term "methyne". E12 shows that the =CH- group is referred to as the methine group. E13 uses the term "methyne" for the same group =CH-. 2,3,4 trimethyl pentane has methine (or methyne) groups. The text at page 2 lines 26 and 57 shows that "t-butyl/methyne" relates to methyne or t-butyl; the wavelength ranges for the two groups overlap.

Experiments with 2,3,4 trimethyl pentane disclosed in the annexes of the letter dated 27 September 1996 show that the third overtone methyne band is at 950-975 nm. and thus outside the wavelengths mentioned in E3.

The authors of E3 did not think of t-butyl/methyne or did not think they mattered. They attribute the preferred wavelengths to certain groups, among which t-butyl/methyne are not mentioned. E3's teaching use of the mentioned groups leads one away from using the methyne band.

VIII. The arguing of Respondent II with respect to the main request is summarised as follows:

According to IUPAC rule A-4.1 and E12 the atom group =C- can be called "methine" group. According to E13 the antiquated notation "methyne" is used for the same atom group. The patent specification does not disclose where the t-butyl/methyne band is situated in the spectrum. The compounds used in the experiments whose results were communicated by the Appellant do not comprise a methyne or methine group.

The compound used in the experiments of the Appellant (2,3,4-trimethyl pentane) is inappropriate since it does not contain a methine group. Moreover the range of the "methyne band" depends on a plurality of parameters.

When using NIR spectroscopy for the determination of properties of substances, appropriate wavelengths can be found with the help of software, furnished by the producer of the devices. The designation of the band is irrelevant; only the use of certain wavelengths is important.

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## Reasons for the Decision

1. The appeal is admissible.
2. *Sufficiency of the disclosure (Article 100(b) EPC)*

The Board sees no reason to call in question the conclusion of the Opposition Division that the ground of Article 100(b) EPC does not prejudice the maintenance of the patent and the arguing of the Division in this respect that the patent specification shows clearly one way to carry out the invention and in particular one wavelength range of the t-butyl/methyne band can be considered suitable for that purpose.

In particular, the allegations with respect to sufficiency of Respondent II that the term "methyne" refers to the =C- group and that the patent does not disclose where the t-butyl/methyne band is situated in the spectrum are not correct. Reference is made also to section 3.2 below.

3. *Main request*
- 3.1 *Ground of opposition laid down in Article 100(c) EPC*

Respondent II, in his statement of grounds of opposition, put forward that the amendment according to the ERRATUM (replacement of "120" on page 6 line 21 by "1230", see section V. above) infringed Article 123(2) EPC. Since the Appellant rescinded said ERRATUM, said objection is null and void.

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3.2 Interpretation of claim 1

3.2.1 The expression "t-butyl/methyne band" is not clear when taking into account the text of claim 1 alone. Does it designate a combination band and/or the t-butyl and the methyne band and/or the methyne or t-butyl band? What does "methyne (band)" mean in the field of analysis of organic compounds with NIR (near infrared range) absorption spectroscopy?

3.2.2 Among the documents cited in this (appeal) decision only E13 (published 1969) and E10 mention the term "methyne". E13 reads:

"**methyne**. The radical  $-CH=$ , attached to 2 different C atoms."

"**methine**. Methenyl:  $HC\equiv$ ."

E10 - published 1986) reads on page 31 lines 28 to 29: "Terminal methylene first overtone bands lie in the region 1611-1636nm (Goddu 1960), and terminal methyne as pent-1-yne 1533 nm."

E15 (published 1979) does not mention "methyne" either; it characterizes the  $HC\equiv$  group by "methylydyne" and adds in a footnote that the group  $=CH-$  may be referred to as the "methine group".

E16 (published 1980) defines the methine group as the diatomic group consisting of one carbon atom and one attached hydrogen and mentions isopentane as an example which contains one methine group. Isopentane does not comprise a double or triple bond. The only group of said compound containing one carbon and one hydrogen atom is the group  $-CH-$  (see Figure 3.090).

E12 (published 1985) mentions under the (German) catchword "Methin" (English: "methine") that according to the IUPAC rule A-4.1 the atom group =CH- can be called methine group. The grouping

HC≡ or -CH- is systematically called "Methylidin".

E7 indicates in chapter "B. Carbon-hydrogen groups" in paragraph 3 of page 638 that "The fundamental carbon-hydrogen stretching vibrations of methyl (CH<sub>3</sub>), methylene (CH<sub>2</sub>), and methine (CH) groups occur at slightly different wavelengths ... The second overtone of the methyl group gives a band at 1.195 μ and that of a methylene group at 1.215 μ ... The corresponding overtone of the methine group appears at 1.225 μ ...". The bands of hydrogen attached to carbon-carbon double and triple bonds are described later on page 641 last paragraph and, respectively, page 642 second paragraph and are not designated by "methine".

In E17 the methine group is only cited in chapter "5.4.1 Alkane" (English: "alkanes") and is cited there after the methylene and methyl groups.

Hence, in the prior art documents on file belonging to the field of IR spectral analysis of organic compounds the term "methyne" is used only in E10 but no clear definition can be derived therefrom, whereas the quite similar term "methine (group)" is repeatedly used. A definition of the term "methyne" is disclosed only in one relatively old chemical dictionary (E13). The meaning of "methine" according to said dictionary is ambiguous when compared with those of the remaining chemical dictionaries. The definitions of "methine" in the documents on file are confusing; the definition according to E7 and E12 complies with the definition of...

"methyne" in E13. It is common to all definitions of both terms that they indicate a radical with only one carbon and only one hydrogen attached only to (a) carbon atom(s). Thus, a clear definition of the term "methyne" cannot be taken from the prior art documents on file.

According to the description of the patent-in-suit the range of (the second overtone of) the methyne band is about 1200 to 1236 nm and comprises thus the band of the (second overtone of) the methine band of E7. According to the description of Example VI the methyne band is obtained from a difference of the spectrum of n-hexane and 2,3,4-trimethyl pentane. None of these compounds contains a C-C multiple bond and the only CH groups of said compounds having only one carbon atom and only one hydrogen atom are the CH groups attached to three different C atoms (hydrogen there being a tertiary hydrogen).

Therefore, the term "methyne" of the patent-in-suit (hereinafter cited between quotation marks) characterizes a radical with one C atom and one - tertiary - H atom attached to three different C atoms.

- 3.2.3 According to the description, the methyne band and the tertiary butyl band overlap (see for example page 2 at the bottom: "The methyne band, along with the tertiary butyl band (1200-1236 nm)... "; page 4 at the bottom: "... the t-butyl/methyne (1212 to 1228) ... "). In the dependent claims (claims 3 and 7) only the composed expression "t-butyl/methyne band" is used. Mention of methyne range/band and a separate t-butyl band and indication of separate wavelength ranges (see page 6 line 22 and page 3 line 49 to 50) in the description suggests that the "t-butyl/methyne band" relates to t-butyl and "methyne".

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Moreover, according to the description the term "band" used in connection with an atom group has a particular meaning in the patent-in-suit: it defines a wavelength range of the (signal indicative of the intensity of the) absorbance or, respectively, of the mathematical function or, respectively, a combination of mathematical functions of said absorbance which is characteristic only for said atom group. Reference is made, e. g., to Figure 3 and 5 and the corresponding description on page 3 lines 44 to 47 and page 6 lines 19 to 22, according to which the wavelength range of the methyne band depends considerably on whether the (signal indicative of the intensity of said) absorbance is used **with** or **without** mathematical treatment. Furthermore, reference is made to page 4 last paragraph and page 6 lines 19 to 22 according to which the wavelength ranges assigned to different atomic groups (methyl, methylene and "t-butyl/methyne" or "methyne") never overlap if they belong to a certain example.

### 3.3 Novelty

It is undisputed that the nearest prior art is disclosed in E3.

Said document teaches that octane numbers can be predicted from absorbance in the range 660-1215 nm. Best correlation between absorbance and octane number is found to occur at 896, 932 and 1164 for research octane number, 930, 940 and 1012 nm for motor octane number and 896, 932 and 1032 nm for pump octane number. These wavelengths are assigned to methyl, methylene or aromatic group C-H vibration bands (see Table I) but not to the "t-butyl/methyne band" in the meaning of the patent-in-suit (see section 3.2.3 above).

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According to the results of the experiments filed by the Appellant, the third overtone of the "methyne band" lies between 950 and 975 nm and outside the third overtone bands of methyl and methylene, namely below 950 nm (see the figure and Maggard's affidavit annexed to the letter dated 27 September 1996), and outside the wavelengths and band used in the third overtone wavelength range of E3, namely 875, 913 and 930-940 nm (see Tables I and II and the paragraph bridging the two columns of page 317). The compounds tested in said experiments - 2-methyl pentane and 2,3,4-trimethyl pentane - do comprise at least one "methyne" group but no double or triple bond, see section 3.2.2 above.

The remaining documents on file are considerably farer away from the subject-matter of claim 1. They do not disclose the use of the "t-butyl/methyne band" in the NIR for the measurement of octane number or the like.

Thus, the subject-matter of claim 1 is novel in the sense of Article 54 EPC.

#### 3.4 Inventive step

The nearest prior art is described in E3 (see section 3.3 above). The subject-matter of claim 1 differs from E3 in that the "t-butyl/methyne band" of the NIR is chosen for the measuring process. Choice of said band effects improvement of the standard error of the octane number (see the examples of the attacked patent). Thus, the problem underlying the subject-matter of claim 1 is to achieve an improvement of said error of the predicted octane number.

E3 stresses the use of methyl, methylene and aromatic CH bands up to 1215 nm (see Table I), since only wavelengths assigned to said bands are used (see the paragraph bridging the two columns of page 317 and

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Table II) and the use of other bands or of wavelengths assigned to the "t-butyl/methyne band" for the purpose of octane number measurement is not recommended there - though the authors of E3 carried out mathematical treatments such as derivatives of the absorbance and multivariate statistics (regression correlations) in the wavelength range comprising the third overtone of the "methyne" band (Figures 1 to 3: 660-1215 nm). Moreover, in view of possible alternatives - analysis of bands of other parts of the IR spectrum (wavelengths above 1215 nm), use of combination bands, C-C vibration bands - use of absorbance in the "t-butyl/methyne band" of the NIR spectrum for the measurement of octane number or the like when taking into account the teaching of E3 alone is not obvious for the skilled person.

Since the remaining documents on file do not disclose the use of the "t-butyl/methyne band" in the NIR for the measurement of octane number or the like, consideration of said documents in combination with E3 by the skilled person cannot lead to the subject-matter of claim 1.

Having regard to the foregoing, the subject-matter of claim 1 involves an inventive step in the sense of Article 56 EPC.

3.5 As a consequence, claim 1 and also the dependent claims, which refer to particular embodiments of claim 1 and thus derive their patentability from claim 1, comply with Articles 52(1) EPC and can be maintained (Article 102(2) EPC).

3.6 Therefore, the main request is allowable.

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4. *Auxiliary requests*

Since the main request is allowable, it is not necessary to deal with the remaining requests.

**Order**

**For these reasons it is decided that:**

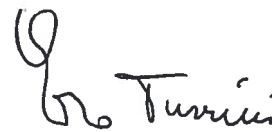
1. The decision under appeal is set aside.
2. The patent is maintained as granted with decision of 29 July 1993, that is without the amendment according to the ERRATUM issued and published on 22 December 1993, having the consequence that the text of the patent specification at the end of line 21 of page 6 reads: "from about 1195-120".

The Registrar:



P. Martorana

The Chairman:



E. Turrini

