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(71) Applicant (for all designated States except US): **SHELL INTERNATIONALE RESEARCH MAATSCHAPPIJ B.V.** [NL/NL]; Carel van Bylandtlaan 30, NL-2596 HR The Hague (NL).

(72) Inventors; and

(75) Inventors/Applicants (for US only): **ARNOLDY, Peter** [NL/NL]; Badhuisweg 3, NL-1031 CM Amsterdam (NL). **BOLINGER, Cornelius, Mark** [US/US]; 514 Oyster Creek Drive, Sugar Land, TX 77478 (US). **DRENT, Eit** [NL/NL]; Badhuisweg 3, NL-1031 CM Amsterdam (NL). **EBERHARD, Michael, Rolf** [DE/GB]; Cantocks Close, Bristol, Avon BS8 1TS (GB). **HEERES, Hero, Jan** [NL/NL]; Badhuisweg 3, NL-1031 CM Amsterdam (NL). **VAN DER LINDEN, Adrianus, Johannes** [NL/NL]; Volmerlanan 8, NI-2288 GD Rijswijk (NL). **MUL, Wilhelmus, Petrus** [NL/NL]; Badhuisweg 3, NI-1031 Cm Amsterdam (NL). **PRINGLE, Paul, Gerard**

[GB/GB]; Cantocks Close, Bristol, Avon BS8 1TS (GB). **SUYKERBUYK, Jacoba, Catherina, Lucia, Johanna** [NL/NL]; Badhuisweg 3, NL-1031 CM Amsterdam (NL). **TAU, Kwoliang, David** [US/US]; 17103 Rolling Brook Ct., Sugar Land, TX 77479 (US).

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Published:

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30 January 2003

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: PROCESS FOR THE CARBONYLATION OF ETHYLENICALLY UNSATURATED COMPOUNDS, BIDENTATE DIPHOSPHINE COMPOSITION USED IN THIS PROCESS AND PROCESSES FOR PREPARATION OF THIS BIDENTATE DIPHOSPHINE COMPOSITION

(57) Abstract: Process for the carbonylation of optionally substituted ethylenically unsaturated compounds by reaction with carbon monoxide and a coreactant in the presence of a catalyst system. The catalyst system includes (a) a source of Pt group metal cations, (b) a bidentate diphosphine composition. More than 60% w/w of bidentate diphosphine present in the bidentate diphosphine composition has the general formula (II) X¹-R-X² wherein X¹ and X² ζ independently represent an optionally substituted symmetrical phosphabicycloalkyl group, having at least 5 ring atoms; and R represents a bivalent organic bridging group, connecting both phosphorus atoms. Bidentate diphosphine composition wherein more than 60% w/w of bidentate diphosphine present has the general formula (II) X¹-R-X² ζ wherein X¹ and X² ζ independently represent an optionally substituted symmetrical phosphabicycloalkyl group, having at least 5 ring atoms; and R represents a bivalent organic bridging group, connecting both phosphorus atoms, with the proviso that the bidentate diphosphine is not 1,3-PP'bis(9-phosphabicyclo[3.3.1]nonyl)propane. In addition methods to prepare such a bidentate diphosphine composition are described.



WO 02/064250 A3

INTERNATIONAL SEARCH REPORT

International Application No
PCT/EP 02/01036

A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 B01J31/24 B01J31/28 C07F9/6568 C07C45/50 C07C29/16
C07F9/50

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC 7 B01J C07F C07C

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, COMPENDEX, INSPEC

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 95 05354 A (SHELL INT RESEARCH ;SHELL CANADA LTD (CA)) 23 February 1995 (1995-02-23) cited in the application page 5, line 2 -page 6, line 15 claims 1,4 8, examples 53,54, table VI	1-4
Y	---	1
P,X	WO 01 87899 A (EBERHARD MICHAEL ROLF ;PRINGLE PAUL GERARD (GB); DRENT EIT (NL); S) 22 November 2001 (2001-11-22) cited in the application page 10, line 1-10 page 10, line 31 -page 11, line 14 page 12, line 15-27 page 16, line 5-25 claims 7-9	1-4
A	page 11, line 15 -page 12, line 6 ---	8,9
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Further documents are listed in the continuation of box C.

Patent family members are listed in annex.

° Special categories of cited documents :

"A" document defining the general state of the art which is not considered to be of particular relevance

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"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search

23 September 2002

Date of mailing of the international search report

23 SEP 2002

Name and mailing address of the ISA

European Patent Office, P.B. 5818 Patentlaan 2
NL - 2280 HV Rijswijk
Tel. (+31-70) 340-2040, Tx. 31 651 epo nl,
Fax: (+31-70) 340-3016

Authorized officer

Goebel, M

INTERNATIONAL SEARCH REPORT

International Application No
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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	GB 2 306 344 A (SHELL INT RESEARCH) 7 May 1997 (1997-05-07) claims 1,6; example 1	1-4
Y	---	1
X	US 5 811 590 A (ARNOLDY PETER ET AL) 22 September 1998 (1998-09-22) claims 1,8; example 1	1-4
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X	EP 0 495 547 A (SHELL INT RESEARCH) 22 July 1992 (1992-07-22) page 9, line 15 -page 10, line 2; claims 1,35	1-4
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X	WO 97 03943 A (SHELL INT RESEARCH ;SHELL CANADA LTD (CA)) 6 February 1997 (1997-02-06) page 5, line 20 - line 26 page 6, line 8 - line 24; claim 6	1-4
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C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X A	US 3 527 818 A (WINKLE JOHN L VAN ET AL) 8 September 1970 (1970-09-08) column 5, line 13-35; claim 3 ---	4 1-3,5-10
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INTERNATIONAL SEARCH REPORT

International application No.
PCT/EP 02/01036

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. Claims Nos.:
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:

3. Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

see additional sheet

1. As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.

2. As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:

4. No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- The additional search fees were accompanied by the applicant's protest.
- No protest accompanied the payment of additional search fees.

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. Claims: 1-3

A process for the carbonylation of olefins and a catalyst system (i) suitable therefor, (i) comprising ligand (ii) and a source of Pt-group metal cations.

2. Claim : 4

A bidentate diphosphine composition wherein more than 60% (w/w) of diphosphine present therein has the general formula II, comprising two symmetrical phosphabicycloalkyl groups, e.g. a suitable ligand (ii) for the catalyst system (i).

3. Claims: 5-7

A process for the separation of any (sic) symmetrical phosphabicycloalkane (SPBA) from mixtures comprising its asymmetrical isomer (APBA), e.g. purification of an intermediate (iii) suitable for the synthesis of ligand (ii).

4. Claims: 8, 9

A process for the preparation of bidentate diphosphines composition wherein more than 60% (w/w) of diphosphine present has the general formula II, e.g. preparation of suitable ligands (ii) for the catalyst system (i) employing intermediates (iii).

5. Claim : 10

A process for the separation of any (sic) bidentate diphosphine (iv) with two symmetrical phosphabicycloalkyl groups (s,s BDP) from a mixtures of bidentate diphosphines comprising said s,s BDP, as well as its mono- and bis-asymmetrical isomers (a,s BDP and a,a BDP, respectively).

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