Precise searching for vaguely defined chemical compounds – what every searcher should know

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ACS International (CAS)

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Table of Contents

- STN Platforms for searching for vaguely defined substances
- Use case “Use of Titanium halide alkoxides in polymerization catalysts for Polypropylene polymerization”:
  - Substructure searching for specific and generic chemical compounds
  - Use of CAS and/or Derwent indexing to improve precision and scope of the search
  - Different ways to combine results from value-added databases
  - Reporting of the search results with 3rd party reporting tools
- Conclusion

STN Platforms appropriate for searching specific and vaguely defined compounds

STN Platform	Biblio-graphic	Specific structures		Generic structures		Advantages/ Disadvantages	
	CAplus/ DWPI	REGISTRY	DCR	MARPAT	DWPIM	Structure editor	Comments
Time coverage	1907- (CAplus) / 1963-/1970- (DWPI)	early 1800s-	1999-/ 2000-	1961-/ 1988-	1961-/ 1987-	-	in case 2 years are stated the first year indicates the first coverage and the latter the full coverage in the database
STN Express	✓	✓	✓	✓	-	+	Best platform for Info Pro's; Best reporting functions
STNext	✓	✓	✓	✓	(✓)*)	++	Comparable to STN Express
new STN	✓	✓	✓	✓	✓	++	Not preferred, only for DWPIM needed
Relevance	✓	✓	Additional use for comprehensive searches; coverage limited (since 1999/'00)	✓	Additional use for com-prehensive searches	Structure editor of New STN + STNext better than the one of STN Express, especially for REGISTRY + MARPAT/DWPIM searches	

*) To be included by Q4/2018 (?)

Use case “Use of Titanium halide alkoxides in polymerization catalysts for Polypropylene polymerization”

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CAS
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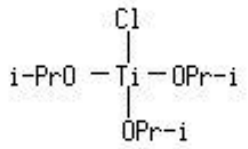
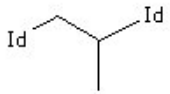
Very precise search keys for very precise answers

RN 20717-86-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Titanium, chlorotris(2-propanolato)-, (T-4)- (CA INDEX NAME)
CN Tris(isopropyloxy)titanium chloride
MF C9 H21 Cl O3 Ti



583 REFERENCES IN FILE CA (1907 T
12 REFERENCES TO NON-SPECIFIC DE
583 REFERENCES IN FILE CAPLUS (19

AN.S DCR-104471
DCSE 104471-0-0-0
CN.P POLY-PROPYLENE
SY HOSTALEN; POLIPROPENE-25; POLY-PROPYLENE; POLYPROPENE;
PP; PROPYLENE,POLY-



CMT A polymer of this structure. Standard polymer
MF Polymer

AN.S DCR-1387
DCSE 1387-0-0-0
CN.P TRI-ISO-PROPOXYTITANIUM CHLORIDE
SY (I-PRO)3TICL; TICL(I-PRO)3; TICL(OPR-I)3;
TRI-ISO-PROPOXYTITANIUM CHLORIDE

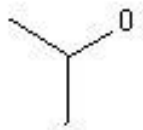
CM 1

Cl

CM 2

Ti

CM 3



CMT 1:1:3 Ratio
MF 3 C3 H8 O . Cl . Ti

Answers in CAS and DWPI for the exactly defined compounds and concepts

Strategy	Registry	CAplus	CApl Patent	Marpat	DCR	WPIX	DWPIM
Specific compounds	633	2,478	1,263		64	236	
Polypropylene	3	276,277	199,696		1	9,839	
Combination1		308	283			3	
PP Man Code						82,491	
PP PLE code						196,930	
Combination2		308	283			47	

Which Derwent manual codes or IPC symbols can be applied to find Titanium halide alkoxides?

- A02-A06B TRANSITION METAL (OXY)HALIDES POLYMERISATION CATALYSTS
- The manual code is not specific to titanium and is also not specific to alkoxides
- For a more precise answer, this aspect would have to be combined to avoid a higher level of noise
- The same is true for the IPC/CPC codes that are available for these broader classes of compounds

  - C08F0004-64 Polymerization catalysts based on Ti, Zr, Hf and their compounds

- For FTO cases, it may be useful to keep the broader answer sets and determine the possible relevancy manually

Answers in CAS and DWPI for the exactly defined compounds and concepts

Strategy	Registry	CAplus	CApl Patent	Marpat	DCR	WPIX	DWPIM
Specific compounds	633	2,478	1,263		64	236	
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PP PLE code						196,930	
Combination2		308	283			47	
TiX-Alk Man code						6,549	
TiOX-plus Ti alkox						698	
Combination3		308	283			146	

Role of Markush databases finding compounds hidden in broader structure disclosures

- The compound could be represented by a Markush-like description in the patent
- That would be the only search option when no specific compounds are exemplified or claimed

(iii) the titanium compound (TC) is of formula (III)

$$(OR')_{4-x}TiCl_x \quad (III)$$

wherein

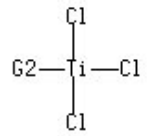
R' is a C_2-C_{20} hydrocarbyl group and

x is an integer of 3 or 4, and

WO2014177480
Borealis

MARPAT

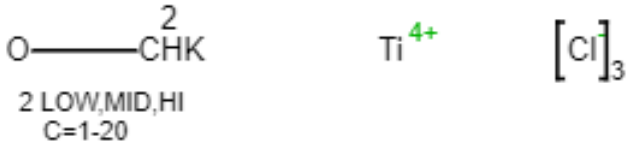
MSTR 2



G2 = hydrocarbyloxy <containing 2-20 C> / Cl /
(Example: OEt)
Patent location: claim 1

DWPIM

1221-92306
Iteration Status: COMPLETE
E: General Chemicals
A: Polymers, Plastics
C: Coordination compounds, Complexes
Y: Mixtures



Expanded results for Markush representation

Strategy	Registry	CAplus	CApl Patent	Marpat	DCR	WPIX	DWPIM
Specific compounds	633	2,478	1,263		64	236	
Polypropylene	3	276,277	199,696		1	9,839	
Combination1		308	283			3	
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PP PLE code						196,930	
Combination2		308	283			47	
TiX-Alk Man code						6,549	
TiOX-plus Ti alkox						698	
Combination3		308	283			146	
Including Markush		1,881	1,881	1,881		1,150	1,446
Markush + Polyprop		601	601			375	
Combination4		786	761			477	

Patents can also represent these compounds in a very vague and textual way not found previously

- There is not enough information given to assign a specific compound identifier
- There is no Markush structure to represent the compound in that way

> The preferred titanium compounds used in the catalyst components of the present invention are $TiCl_4$ and $TiCl_3$; furthermore, also Ti-haloalcoholates of formula $Ti(OR)_{n-y}X_y$, where n is the valence of titanium and y is a number between 1 and n, can be used.

WO2005123784
Basell Poliolefine

11. 权利要求4的乙烯-α -烯烃共聚物的制造方法，其中所述IV B族金属化合物选自IV B族金属卤化物、IV B族金属烷基化合物、IV B族金属烷氧基化合物、IV B族金属烷基卤 化物和IV B族金属烷氧基卤化物中的一种或多种，优选选自IV B族金属卤化物中的一种或 多种，更优选选自TiCl4、TiBr4、ZrCl4、ZrBr4、HfCl^P HfBr4中的一种或多种，最优选选自 TiCl4 ZrCl4中的一种或多种，所述错氧烧选自甲基错氧烧、乙基错氧烧、异丁基错氧烧和 正丁基错氧烧中的一种或多种，更优选选自甲基错氧烧和异丁基错氧烧中的一种或多种，而所述烧基错选自二甲基错、乙基错、丙基错、二异丁基

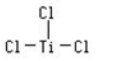
The method for producing an ethylene-α-olefin copolymer according to claim 4, wherein said Group IV B metal compound is selected from the group consisting of One or more of a Group IV B metal halide, a Group IV B metal alkyl compound, a Group IV B metal alkoxide, a Group IV B metal alkyl halide, and a Group IV B metal alkoxy halide, It is preferably one or more selected from the group IV B metal halides, more preferably one or more selected from the group consisting of TiCl4, TiBr4, ZrCl4, ZrBr4, HfCl^P HfBr4, most preferably one selected from the group consisting of TiCl4

CN 105001360
Sinopec

There are 9 cases where titanium halides form compounds with alcohols

RN 18807-23-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanol, compd. with titanium chloride (TiCl3) (5:1) (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Titanium chloride (TiCl3), compd. with methanol (1:5) (8CI)
MF **C H4 O . 1/5 Cl3 Ti**
SR CA
LC STN Files: CA, CAPLUS

CRN 7705-07-9
CMF Cl3 Ti



CM 2

CRN 67-56-1
CMF C H4 O

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Finding index terms for more vaguely defined compounds

- Showing CA Lexicon as a source for vague description of the organometallic compound or the polymer

```
E124     16665   BT5  Chemical compounds/CT
E125     10259     BT4  Transition metal compounds/CT
E126      1982       BT3  Transition metal salts/CT
E127       114         BT2  Transition metal alkoxides/CT
E128      1117           BT1  Group 4 element alkoxides/CT
E129         0              -->  Titanium isopropoxide/CT
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E183     16665   BT4  Chemical compounds/CT
E184     21396     BT3  Halides/CT
E185     16665   BT4  Chemical compounds/CT
E186     10259     BT3  Transition metal compounds/CT
E187      1634       BT2  Transition metal halides/CT
E188       917         BT1  Transition metal chlorides/CT
E189         0           -->  Titanium tetrachloride/CT
```

What base compounds and concepts could be considered ?

- Titanium linked with alkoxy and halo (chloro, bromo, fluoro) derivatives
- Specific Titanium alkoxides linked with halo derivatives
- Specific Titanium halides linked with alkoxy derivatives

- Titanates/CT linked with halo derivatives
- Metal alkoxides/CT linked with halo derivatives
- Group 4 element alkoxides/CT linked with halo derivatives
- Transition metal alkoxides/CT linked with halo derivatives
- Transition metal halides/CT linked with alkoxy derivatives
- Transition metal chlorides/CT linked with alkoxy derivatives

Final answers of combinations of Titanium halide alkoxides and polypropylene in CAS and WPI files

Strategy	Registry	CAplus	CApl Patent	Marpat	DCR	WPIX	DWPIM
Specific compounds	633	2,478	1,263		64	236	
Polypropylene	3	276,277	199,696		1	9,839	
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Combination3		308	283			146	
Including Markush		1,881	1,881	1,881		1,150	1,446
Markush + Polyprop		601	601			375	
Combination4		786	761			477	
Vague TiXAlk		102	66			-	
Combination5		786	761			477	
Unique Answers			627			348	

Different ways to combine searches from two value-added databases

- The patents indexed with titanium halide alkoxides, either specific, Markush or textual generic have been combined with polypropylene in each of the file groups
- Simple cross-file searching of patent numbers with kind codes (PNK) was done to examine unique answers for each of the databases CAplus and WPIX.
- There is clearly an advantage in the use of specific CAS Registry numbers for compounds in CAS files and the thorough indexing of polymers with Derwent polymer codes or manual codes.
- Would there be patent documents that would have a specific CAS RN for a titanium halide alkoxide indexed in CAplus and a polymer code in WPIX which are not available in the currently retrieved combination for each file?
- Crossing over the patent documents for the CAS RNs of Titanium halide alkoxide that do not have polypropylene indexed in CAplus to WPIX gave an opportunity to combine this list with the polymer code in WPIX excluding where the Ti compound was indexed in WPIX.

Example of 12 unique hits WO2009058930

Polymer Product

[0036] The polymers (and blends thereof) formed via the processes described herein may include, but are not limited to, linear low density polyethylene, elastomers, plastomers, high density polyethylenes, low density polyethylenes, medium density polyethylenes, polypropylene (*e.g.*, syndiotactic, atactic and isotactic) and polypropylene copolymers, for example.

[0049] The preparation then included adding 100 mmol (77.5 g) of $ClTi(O^iPr)_3$ (1M in hexane) to the mixture at room temperature over 30 minutes. A clear, solid free solution (reaction mixture "A") was obtained. The reaction mixture "A" was then stirred at room temperature for another hour.

- Polypropylene not indexed in CAplus
- ClTi(OPr)3 not indexed in WPIX

Reporting of the search results with 3rd party reporting tools

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Overview of STN searching and reporting tools

STNext or STN Express

- Analyze and Display Patent numbers

new STN

- Q term list
- *DWPIM → DWPI*
- Structure + indexing display from HCAplus

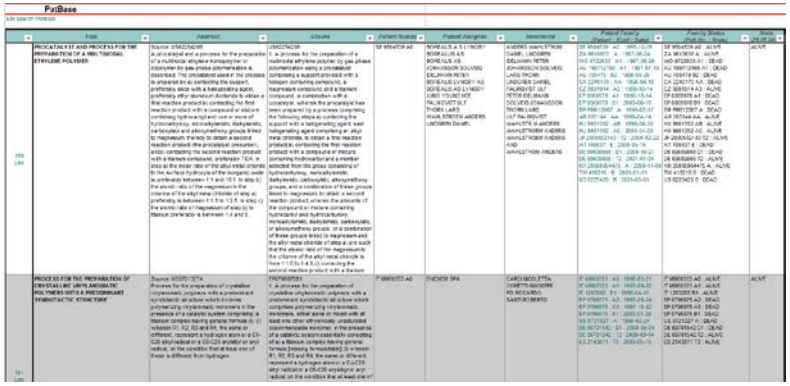
PatBase

- BIB data with abstracts and claims;
- Patent family and legal status information

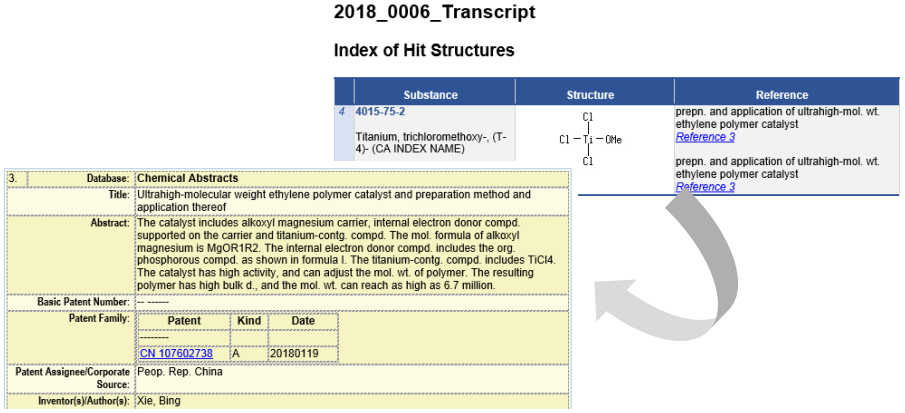
BizInt Smart Charts for Patents

Reporting via a 3rd party tool:
e. g.
- *BizInt Smart Charts for Patents*
- *PatSeer Projects*

i) "Dead or Alive" *BizInt*-Excel-Report



ii) *BizInt*-Word-Report with Hit-structure:



2018_0006_Transcript

Index of Hit Structures

	Substance	Structure	Reference
4	4015-75-2 Titanium, trichloromethoxy-, (T-4)- (CA INDEX NAME)	Cl Cl—Ti—OMe Cl	prepn. and application of ultrahigh-mol. wt. ethylene polymer catalyst Reference 3

3.	Database:	Chemical Abstracts
	Title:	Ultrahigh-molecular weight ethylene polymer catalyst and preparation method and application thereof
	Abstract:	The catalyst includes alkoxyl magnesium carrier, internal electron donor compd. supported on the carrier and titanium-contg. compd. The mol. formula of alkoxyl magnesium is MgOR1R2. The internal electron donor compd. includes the org. phosphorous compd. as shown in formula I. The titanium-contg. compd. includes TiCl4. The catalyst has high activity, and can adjust the mol. wt. of polymer. The resulting polymer has high bulk d., and the mol. wt. can reach as high as 6.7 million.
	Basic Patent Number:	---
	Patent Family:	Patent: CN 107602738 / Kind: A / Date: 20180119
	Patent Assignee/Corporate Source:	Peop. Rep. China
	Inventor(s)/Author(s):	Xie, Bing

BizInt-Report (1/2)

Excel (optimized HTML) with Patent family and Legal status information (from PatBase) and patent full-text linking

Record link to FIZ AutoDoc

PatBase

SIM Search Protocol

	Title	Abstract	Claims	Patent Numbe	Patent Assignee	Inventor(s)	Patent Family (Patent : Kind : Date)	Family Status (Pub No. : State)	State (25.07.20
150 Link	PROCATALYST AND PROCESS FOR THE PREPARATION OF A MULTIMODAL ETHYLENE POLYMER	Source: US6225420B A procatalyst and a process for the preparation of a multimodal ethylene homopolymer or copolymer by gas-phase polymerisation is described. The procatalyst used in the process is prepared by:a) contacting the support, preferably silica with a halogenating agent, preferably ethyl aluminium dichloride to obtain a first reaction product,b) contacting the first reaction product with a compound or mixture containg hydrocarbyl and one or more of hydrocarbyloxy, monoalkylamido, dialkylamido, carboxylato and alkoxymethoxy groups linked to magnesium, thereby to obtain a second reaction product (the procatalyst precursor), andc) contacting the second reaction product with a titanium compound, preferably TiCl4. In step a) the molar ratio of the alkyl metal chloride to the surface hydroxyls of the inorganic oxide is preferably between 1:1 and 10:1. In step b) the atomic ratio of the magnesium to the chlorine of the alkyl metal chloride of step a) preferably is between 1:1.5 to 1:2.5. In step c) the atomic ratio of magnesium of step b) to titanium preferably is between 1.4 and 5.	US6225420B 1. A process for the preparation of a multimodal ethylene polymer by gas-phase polymerization using a procatalyst comprising a support provided with a halogen containing compound, a magnesium compound and a titanium compound, in combination with a cocatalyst, wherein the procatalyst has been prepared by a process comprising the following steps:a) contacting the support with a halogenating agent, said halogenating agent comprising an alkyl metal chloride, to obtain a first reaction product,b) contacting the first reaction product with a compound or mixture containing hydrocarbyl and a member selected from the group consisting of hydrocarbyloxy, monoalkylamido, dialkylamido, carboxylato, alkoxymethoxy groups, and a combination of these groups linked to magnesium, to obtain a second reaction product,wherein the amounts of the compound or mixture containing hydrocarbyl and hydrocarbyloxy, monoalkylamido, dialkylamido, carboxylato, or alkoxymethoxy groups, or a combination of these groups linked to magnesium and the alkyl metal chloride of step a) are such that the atomic ratio of the magnesium to the chlorine of the alkyl metal chloride is from 1:1.0 to 1:4.0,c) contacting the second reaction product with a titanium	SE 9504539 A0	BOREALIS A S LYNGBY BOREALLIS AS BOREALIS AS JOHANSSON SOLVEIG IDELMANN PETER BOREALIS LYNGBY AS BOREALIS AS LYNGBY JUNG YOUNG HEE PALMQVIST ULF THORN LARS WAHLSTROEM ANDERS LINDGREN DANIEL	ANDERS WAHLSTROM DANIEL LINDGREN IDELMANN PETER JOHANSSON SOLVEIG LARS THORN LINDGREN DANIEL PALMQVIST ULF PETER IDELMANN SOLVEIG JOHANSSON THORN LARS ULF PALMQVIST WAHLSTR M ANDERS WAHLSTROEM ANDERS WAHLSTROEM ANDERS AND WAHLSTROM ANDERS	SE 9504539 : A0 : 1995-12-19 ZA 9610637 : A : 1997-06-24 WO 9722633 : A1 : 1997-06-26 AU 199712166 : A1 : 1997-07-14 AU 705479 : B2 : 1999-05-20 CA 2240170 : AA : 1998-06-10 CZ 9801914 : A3 : 1998-10-14 EP 0869978 : A1 : 1998-10-14 EP 0869978 : B1 : 2000-08-16 BR P9612067 : A : 1999-02-17 AR 005144 : AA : 1999-04-14 HU 9901352 : AB : 1999-08-30 HU 9901352 : AC : 2000-04-28 JP 2000502143 : T2 : 2000-02-22 AT 195537 : E : 2000-09-15 DE 69609865 : D1 : 2000-09-21 DE 69609865 : T2 : 2001-01-04 KR 20000064475 : A : 2000-11-06 TW 418216 : B : 2001-01-11 US 6225420 : B : 2001-05-01	SE 9504539 A0 : ALIVE ZA 9610637 A : ALIVE WO 9722633 A1 : DEAD AU 199712166 A1 : DEAD AU 705479 B2 : DEAD CA 2240170 AA : DEAD CZ 9801914 A3 : ALIVE EP 0869978 A1 : DEAD EP 0869978 B1 : DEAD BR P9612067 A : DEAD AR 005144 AA : ALIVE [illegible] : ALIVE HU 9901352 AC : ALIVE JP 2000502143 T2 : ALIVE AT 195537 E : DEAD DE 69609865 D1 : DEAD DE 69609865 T2 : ALIVE KR 20000064475 A : ALIVE TW 418216 B : DEAD US 6225420 B : DEAD	ALIVE
151 Link	PROCESS FOR THE PREPARATION OF CRYSTALLINE VINYLAROMATIC POLYMERS WITH A PREDOMINANT SYNDIOTACTIC STRUCTURE	Source: US5721327A Process for the preparation of crystalline vinylaromatic polymers with a predominant syndiotactic structure which involves polymerizing vinylaromatic monomers in the presence of a catalytic system comprising: a titanium complex having general formula (I): (I) wherein R1, R2, R3 and R4, the same or different, represent a hydrogen atom or a C1-C20 alkyl radical or a C6-C20 arylalkyl or aryl radical, on the condition that at least one of these is different from hydrogen.	EP0796875B1 1. A process for the preparation of crystalline vinylaromatic polymers with a predominant syndiotactic structure which comprises polymerizing vinylaromatic monomers, either alone or mixed with at least one other ethylenically unsaturated copolymenzable monomer, in the presence of a catalytic system essentially consisting of a) a titanium complex having general formula [missing formula/table] (I) wherein R1, R2, R3 and R4, the same or different, represent a hydrogen atom or a C4-C20 alkyl radical or a C6-C20 arylalkyl or aryl radical, on the condition that at least one of	IT MI960553 A0	ENICHEM SPA	CARDI NICOLETTA COMETTI GIUSEPPE PO RICCARDO SANTI ROBERTO	IT MI960553 : A0 : 1996-03-21 IT MI960553 : A1 : 1997-09-22 IT 1283282 : B1 : 1998-04-16 EP 0796875 : A2 : 1997-09-24 EP 0796875 : A3 : 1997-10-22 EP 0796875 : B1 : 2000-03-29 US 5721327 : A : 1998-02-24 DE 69701542 : D1 : 2000-05-04 DE 69701542 : T2 : 2000-09-14 ES 2143811 : T3 : 2000-05-16	IT MI960553 A0 : ALIVE IT MI960553 A1 : ALIVE IT 1283282 B1 : ALIVE EP 0796875 A2 : DEAD EP 0796875 A3 : DEAD EP 0796875 B1 : DEAD US 5721327 A : DEAD DE 69701542 D1 : DEAD DE 69701542 T2 : ALIVE ES 2143811 T3 : ALIVE	ALIVE

Legal status information with DEAD or ALIVE flag

Patent family information with Patent full-text link (e. g. to Espacenet or Patent Order Direct)

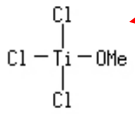
BizInt-Report (2/2)

Word (Summary Record format) with Hit-structure

2018_0006_Transcript

Index of Hit Structures

Structures with annotations

	Substance	Structure	Reference
4	4015-75-2 Titanium, trichloromethoxy-, (T-4)- (CA INDEX NAME)		prepn. and application of ultrahigh-mol. wt. ethylene polymer catalyst *Reference 3* prepn. and application of ultrahigh-mol. wt. ethylene polymer catalyst *Reference 3*

Each hit substance identified

Link to references for each structure

3.	Database:	Chemical Abstracts
	Title:	Ultrahigh-molecular weight ethylene polymer catalyst and preparation method and application thereof
	Abstract:	The catalyst includes alkoxyl magnesium carrier, internal electron donor compd. supported on the carrier and titanium-contg. compd. The mol. formula of alkoxyl magnesium is MgOR1R2. The internal electron donor compd. includes the org. phosphorous compd. as shown in formula I. The titanium-contg. compd. includes TiCl4. The catalyst has high activity, and can adjust the mol. wt. of polymer. The resulting polymer has high bulk d., and the mol. wt. can reach as high as 6.7 million.
	Basic Patent Number:	-- ------
	Patent Family:	Patent / Kind / Date -------- / / CN 107602738 / A / 20180119
	Patent Assignee/Corporate Source:	Peop. Rep. China
	Inventor(s)/Author(s):	Xie, Bing

Patent full-text link

Conclusion

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Conclusion

What you have to consider for the search for vaguely defined chemical substances (in the present case metal organic compounds and polymers).

- Use index-assisted searches for chemical names in REGISTRY and controlled terms in CAplus to include different designations for vaguely defined chemical substances.
- Be aware of the different indexing policies of CAS and Derwent in (substructure) searches for metal organic compounds: CAS indexes as complete substance (e. g. X-Ti-O-Alk), Derwent by its separate ions (e. g. X + Ti + O-Ak).
- Use crossfile searching to make use of the best indexing from each vendor and to find results where only a part is indexed by the vendor (e. g. the substance at CAS and the polymer at Derwent).
- 3rd party reporting tools (e. g. *BizInt* or *PatSeer Projects*) can bring additional value to the client by including legal status information and patent full-text linking or by adding structure display with bibliographic linking.

Thank you very much for your attention!

Any questions?

klaus.walden@clariant.com
ppeters@acs-i.org