

CAS STNEXT® WEBINAR

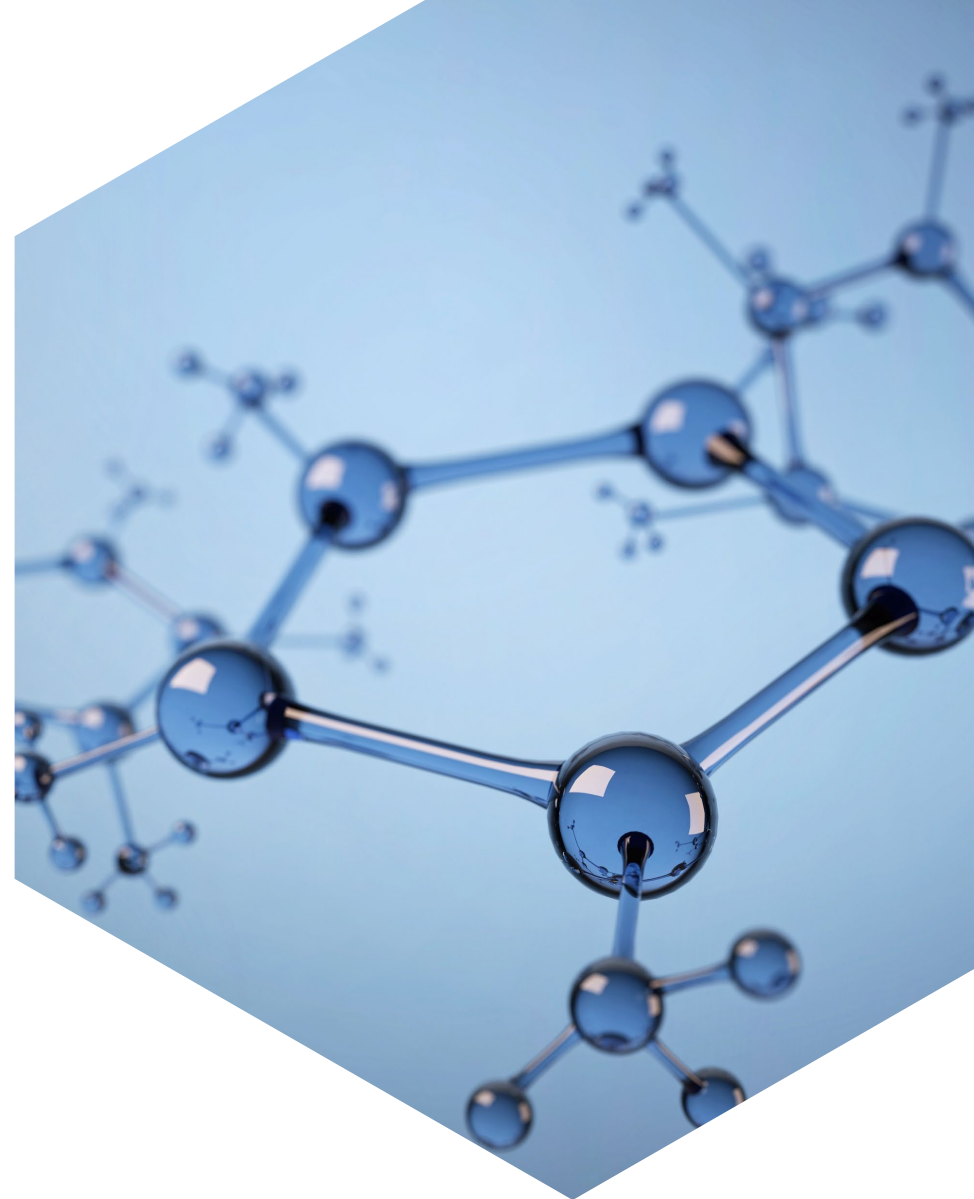
HOW TO SEARCH COORDINATION COMPOUNDS IN CAS STNEXT

Dr. Larissa Bergmann – FIZ Karlsruhe

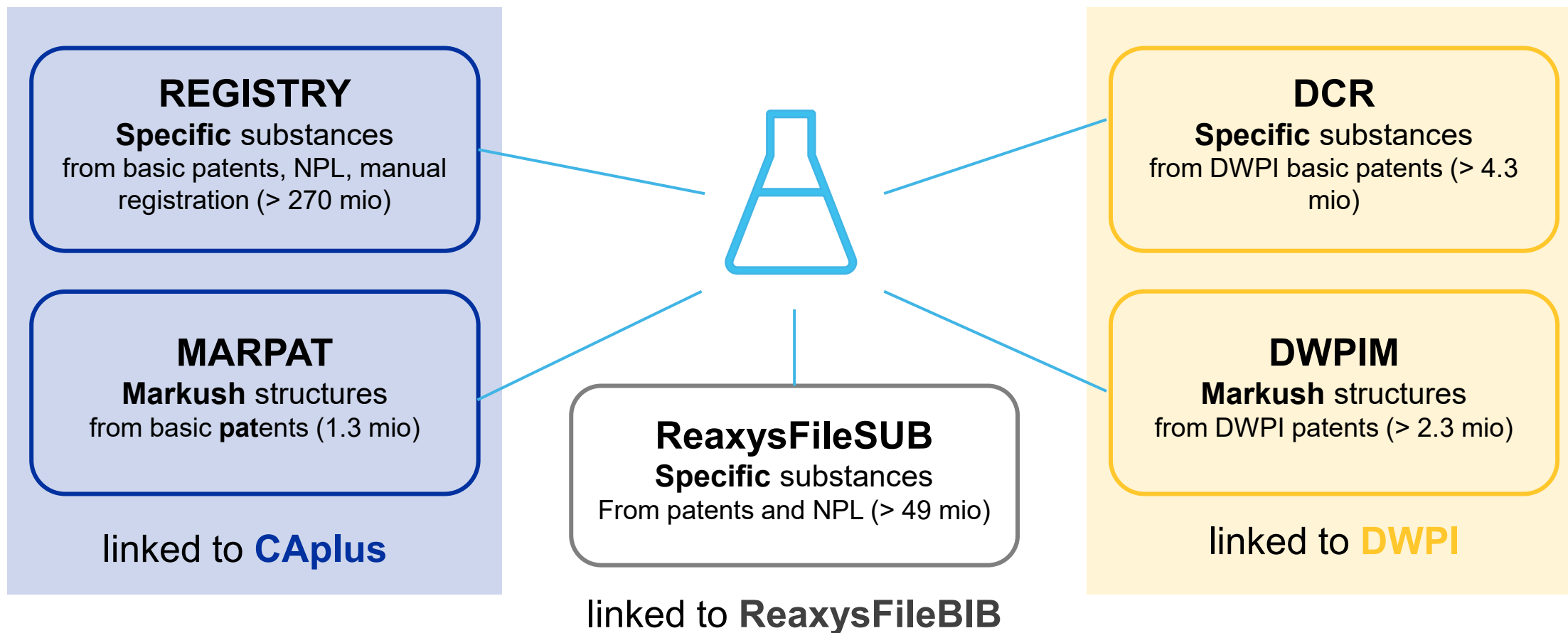
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AGENDA

- Introduction
- Search coordination compounds:
 - In CAS files
 - In Derwent files
 - In Elsevier files
- Summary

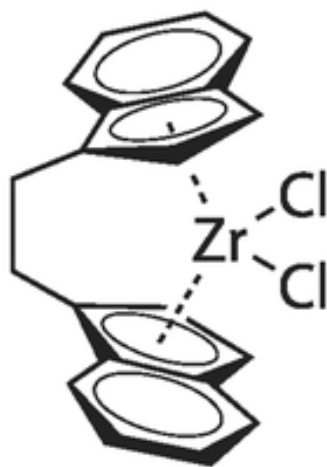


Essential substance databases in CAS STNext



Example – Kaminsky catalyst

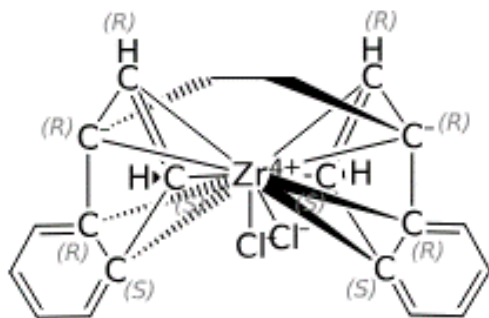
for olefin polymerization



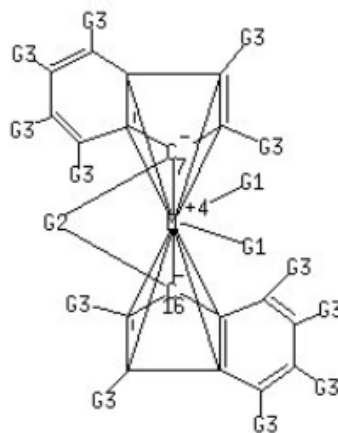
rac-1,2-Ethylenebis(indenyl)zirconium dichloride

Indexing rules vary between files

CAS REGISTRY (RN 100080-82-8)



MARPAT



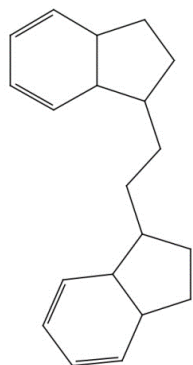
G2 = CH₂ (opt. substd.)
G13 = Zr

Patent location: claim 13

G13

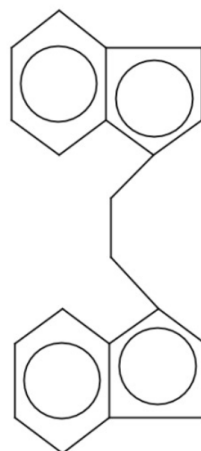
DCR (DCR-210988)

CM 1 CM 2 3

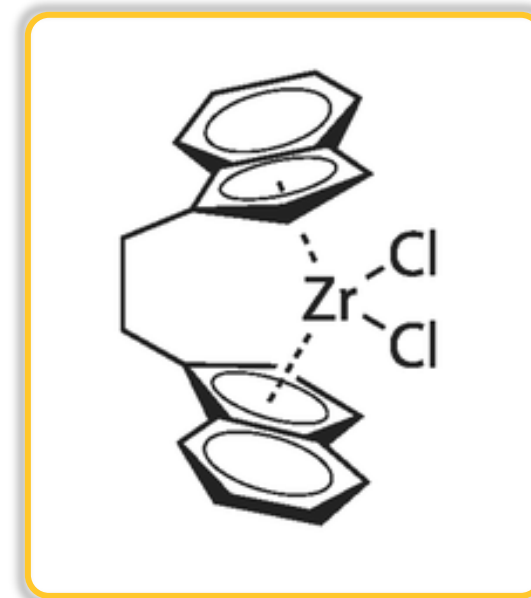


Zr Cl⁻

DWPIM

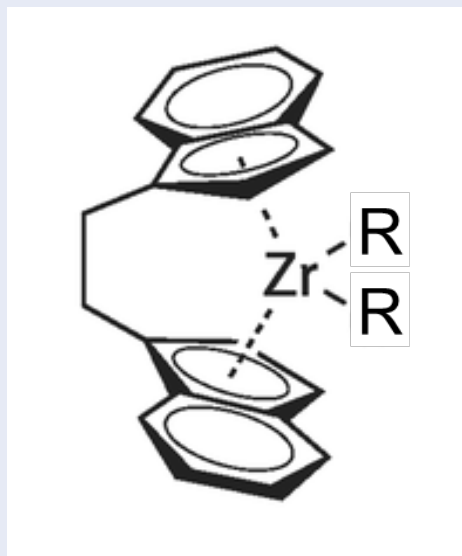


Zr^{2+, 2} [Cl]₂



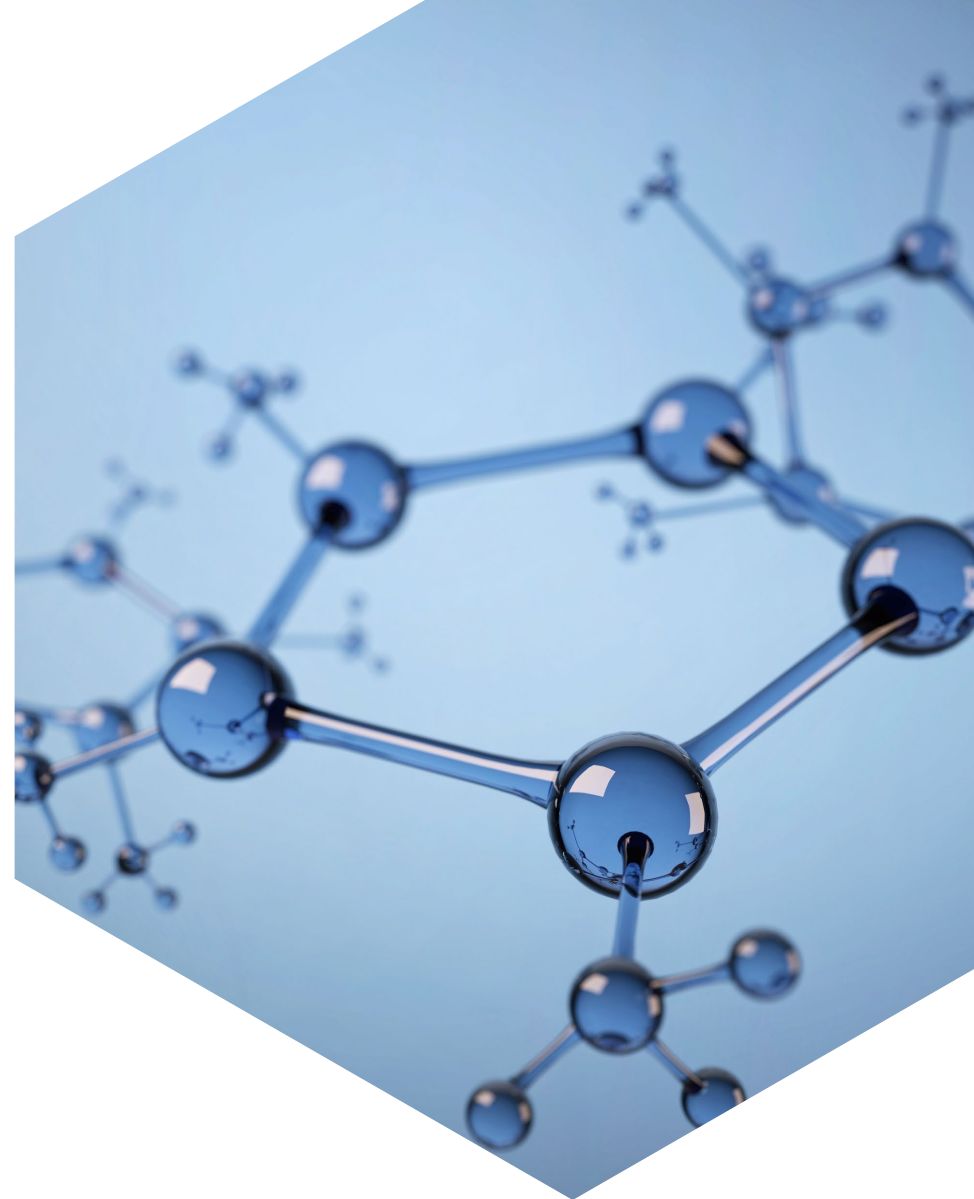
Example – Coordination compound search

Find zirconium coordination compounds containing two indenyl ligands, linked by an ethylene bridge.



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 - **In CAS files**
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REGISTRY record for a coordination compound

CAS Registry Number:

100080-82-8 REGISTRY

Entered STN: 01 Feb 1986

CAS Registry Number Locator:

STN Files: CA, CAPLUS, CASFORMULTNS, CASREACT, CHEMCATS, CHEMLIST, TOXCENTER, [View all](#)

Chemical Name:

Zirconium, dichloro[rel-(7aR,7'aR)-1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]- (CA INDEX NAME)

OTHER CA INDEX NAMES:

Dichloro[rel-(7aR,7'aR)-1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]zirconium

Zirconium, dichloro[1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]-, stereoisomer

OTHER NAMES:

Rac-(ethylenebis(η5-1-indenyl))dichlorozirconium
rac-1,2-Ethylidenebis(1-indenyl)zirconium dichloride
rac-Dichloro[1,2-ethylenebis(1-indenylidene)]zirconium

Rac-ethylenebis(η5-1-indenyl)zirconium dichloride

[View all](#)

Class Identifier:

CCS

File Segment:

STEREOSEARCH

Molecular Formula:

C20 H16 Cl2 Zr

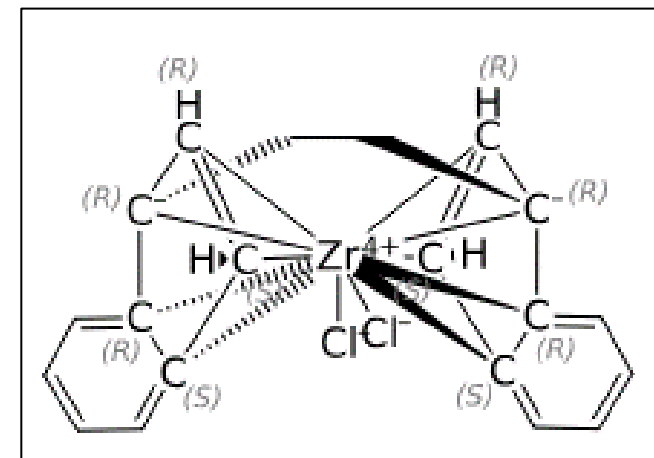
Source of Registration:

CA

1056 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1059 REFERENCES IN FILE CAPLUS (1907 TO DATE)



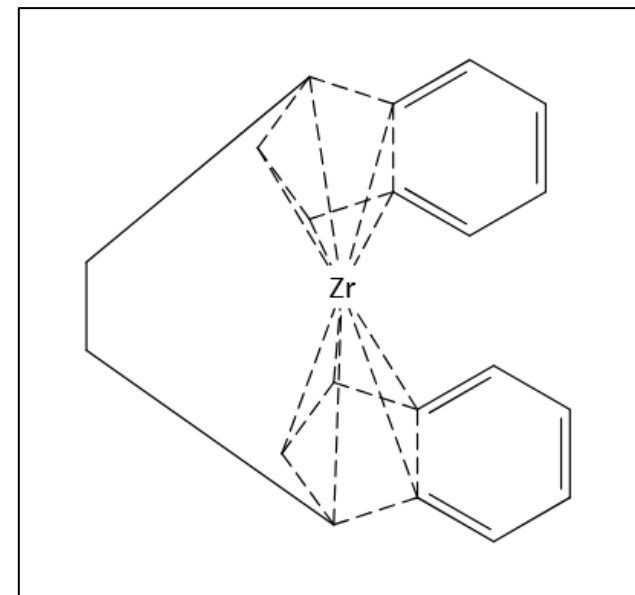
A coordination compound comprises a central metal atom which has a number of bonds attached that is not equal to its valence.

Guidelines for coordination structure queries in REGISTRY

Prepare structure with **unspecified bonds** for ligand

1. Draw structure
 - Draw a bond from metal to any potentially coordinating atom
 - Use **unspecified** bonds
 - Do **not block ring fusion**
 - Do not specify charges
2. Upload structure
3. Perform SSS SAMple search, scan retrieved structures and revise structure query if necessary
4. Perform SSS FULL

→ Search ligand and Zr with coordination bonds:

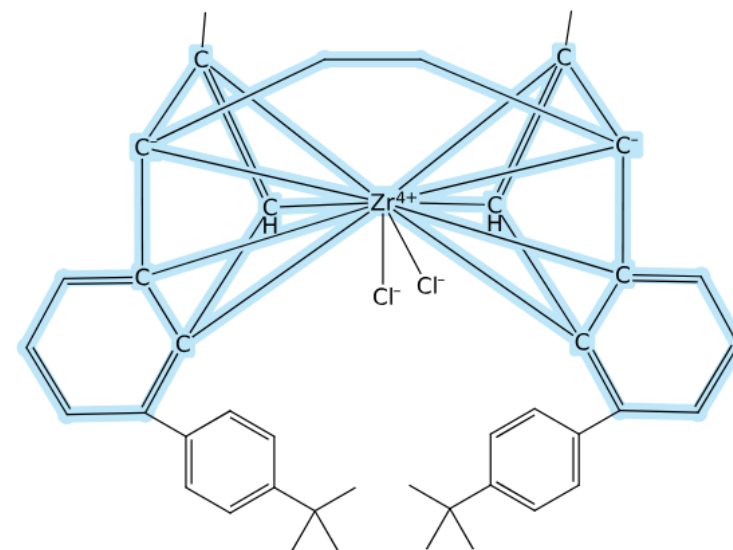
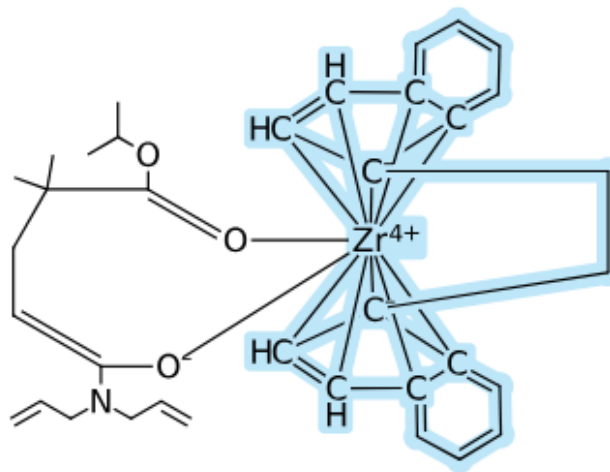
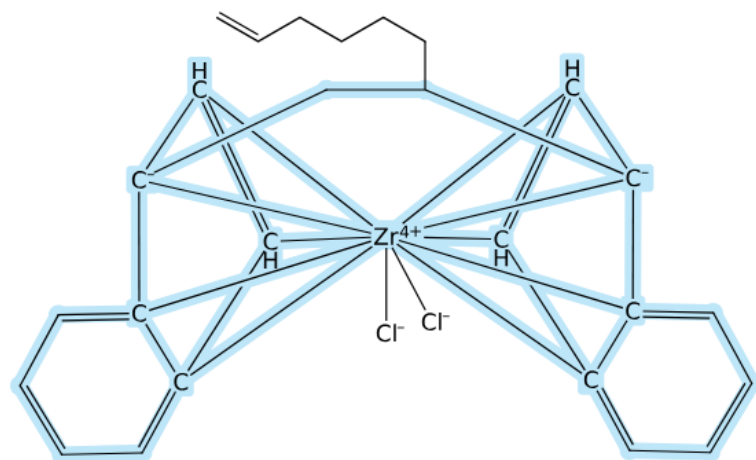


Note: If metal coordination is left open, remember to assign RING/CHAIN to all chain bonds of ligand!

Retrieved records - REGISTRY

917 results

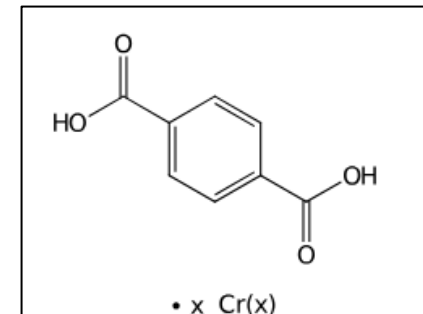
*Search performed on 20250912



Consider other search options - REGISTRY

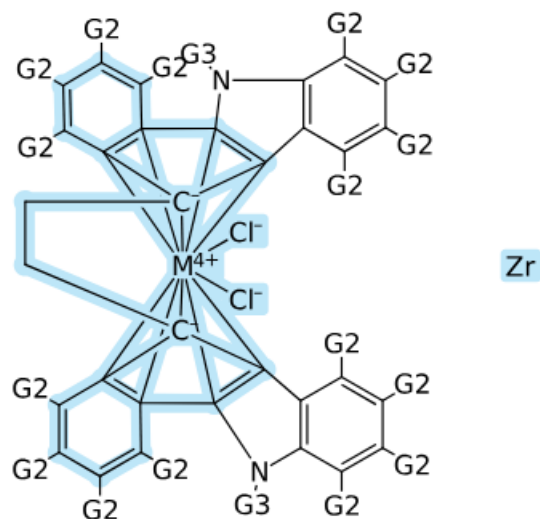
Also consider to search for coordination compounds:

- indexed as salts:
 - Search for ligand by structure, refine by Zr/ELS
 - Do not restrict to CCS/CI
- in the editor's note field **/ENTE**:
 - used for trade name manual registrations
 - Free text form
e.g. => S (?poly? and zirconium)/ENTE



```
RN 1415808-42-2  REGISTRY
ED Entered STN: 02 Jan 2013
CN Orgatix TZ 150  (CA INDEX NAME)
ENTE A zirconium-based polymerization catalyst (Matsumoto Fine Chemical Co., Ltd.)
MF Unspecified
CI MAN
SR CA
LC STN Files:  CA, CAPLUS, USPAT2, USPATFULL
          3 REFERENCES IN FILE CA (1907 TO DATE)
          3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
```

MARPAT records for a coordination compound



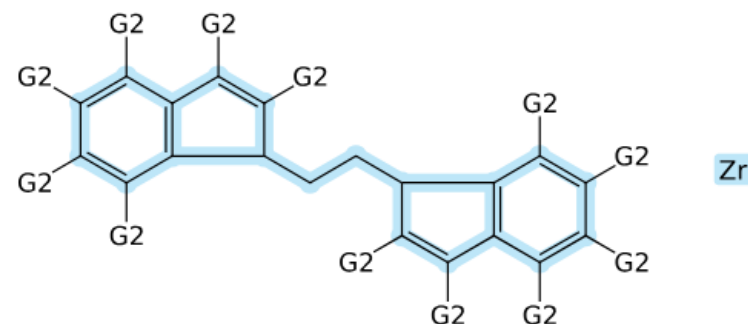
Patent location:

claim 1

Note:

substitution is restricted

A coordination compound can be indexed with central M-node with bonds to the ligand(s) (not equal to the metal's valence), and a specific Zr as separate fragments.



Patent location:

claim 5

Note:

as complexes with G10

Note:

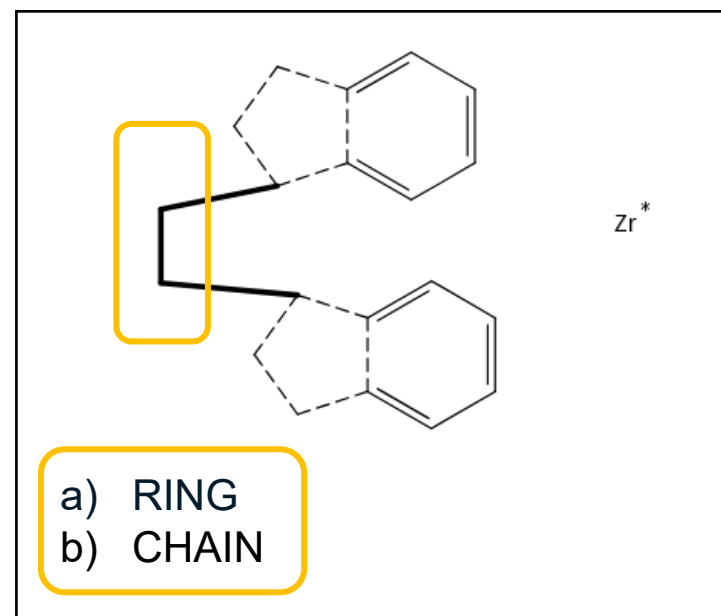
additional ligands and dimers also claimed

A coordination compound can also be indexed as the Markush structure of the ligand with Zr as a separate fragment, without metal-ligand bonds defined.

Guidelines for coordination structure queries in MARPAT

1. Draw ligand
 - Use unspecified bonds
 - Assign Match level ATOM to all potentially coordinating atoms from ligand
 - Do not block ring fusion
2. Draw specific metal as separate fragment
 - Leave the node type CHAIN.
 - Assign Match level ATOM
3. **Use 2 structure queries for this ligand:**
 - a. Assign **RING** for bonds and atoms of ligand's bridge
 - b. Assign **CHAIN**
4. Perform SSS SAMPLE search, scan retrieved structures (D SCAN FQHIT) and revise structure query if necessary
5. Perform SSS FULL

→ Search ligand and Zr as separate fragments:

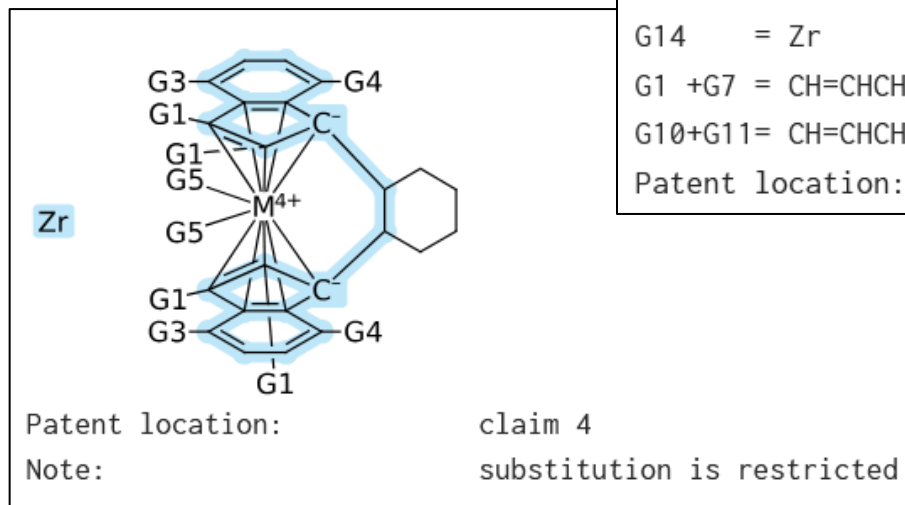
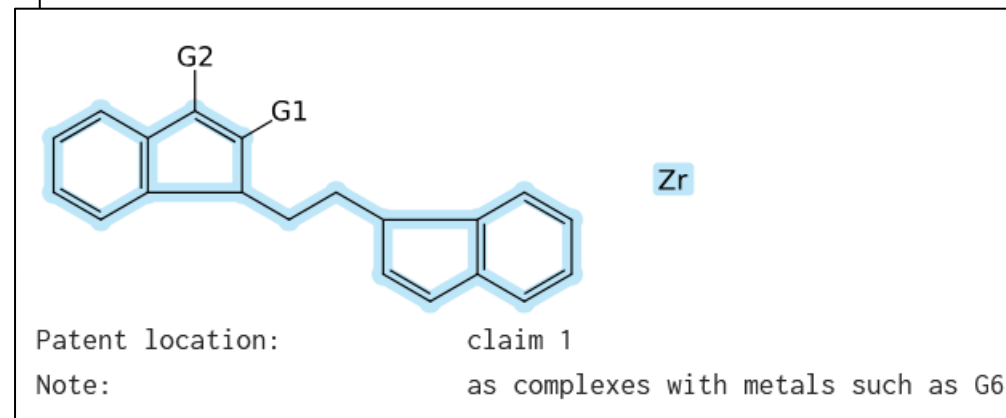
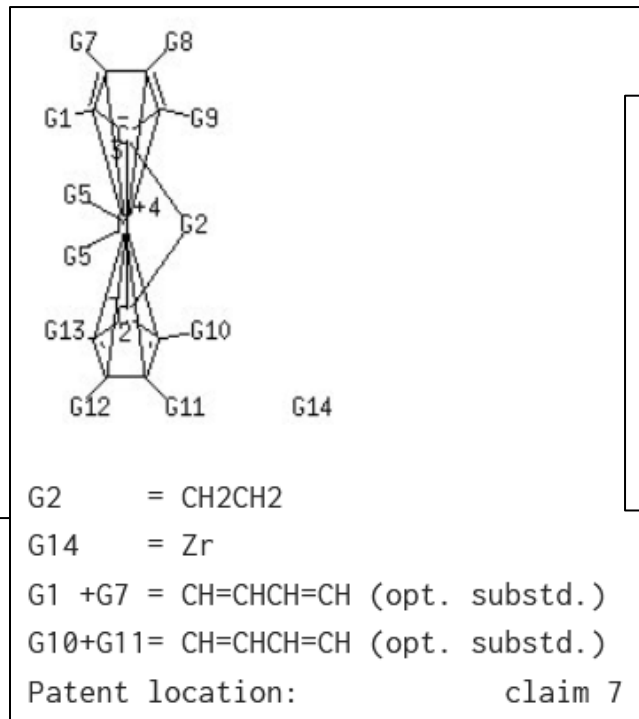
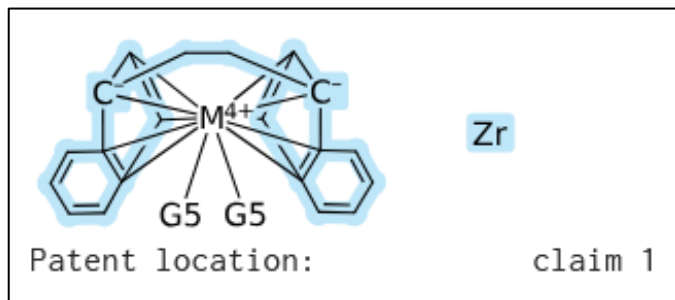


Retrieved records - MARPAT

1046 results

*Search performed on 20250912

=> d scan FQHIT

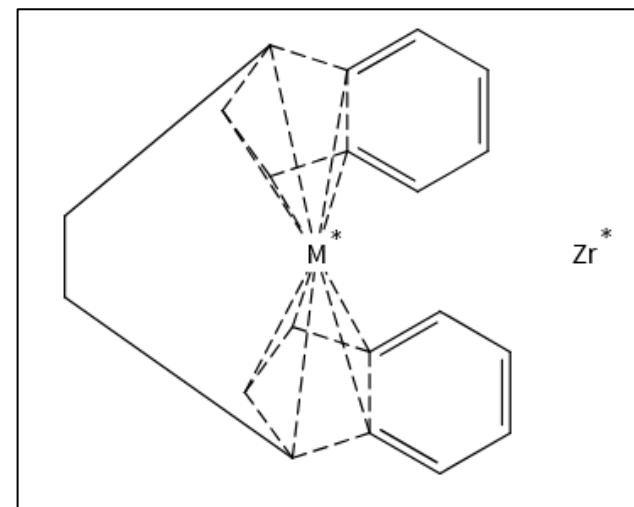


Increase precision in structure query

Defined M→ligand coordination

1. Draw ligand with metal coordination:
 - Use the variable “M” node for the metal atom(s). Draw a bond from M to any potentially coordinating atom.
 - Use **unspecified** bonds
 - Do **not block ring fusion**, do not specify charges.
2. Draw the specific metal(s) as a separate fragment(s).
 - Leave the Node Characteristic as CHAIN.
3. Assign Match levels:
 - **CLASS** to **M**-node
 - **ATOM** to **specific metal** fragment
 - **ATOM** to potentially coordinating atoms from **ligand**

→ Define metal-ligand bonds:



Bibliographic database HCAplus

1. Crossover REG and MARPAT results to HCAplus, refine by document type, key words or roles, and review
2. Consider other search options in HCAplus:
 - **Search for chemical names of specific compounds in non-indexed records**
 - **Search for substance class name**
 - Consider CAS Lexicon as source for keyword searching
 - **Search for complexes as „derivatives of ligand(s)“ via RN of ligands**
 - **Search CASREACT:**
 - **Unique hits that are indexed in reactions, but not in substances in Caplus record**

Bibliographic database HCAplus

Add search precision by Roles

=> S HELP ROLES

...

=> E CAT+ALL/RL

E1 20799589 BT1 Uses/RL

E2 2325485 --> CAT/RL

E3 2325485 Catalyst Use/RL

NOTE vol. 66 (1967) to present - Assigned to a substance where there is a demonstrated, claimed, or clearly intended use as a promoter, initiator, or functional equivalent in any reactions or processes on a lab or

=> S L3 (L) CAT/RL

L4 2382 L3 (L) CAT/RL

Crossover from REGISTRY

=> D SCAN

TI Preparation of (2-indenyl)(1-indenyl)transition metal complexes as olefin polymerization catalysts and method of producing olefin polymer

...

IT 100-99-2, Triisobutylaluminum, uses [112243-78-4](#),
Ethylenebis(1-indenyl)zirconium dichloride 119821-97-5,
Dimethylsilylenebis(1-indenyl)zirconium dichloride 128178-27-8
1009111-01-6

RL: [CAT \(Catalyst use\)](#): USES (Uses)

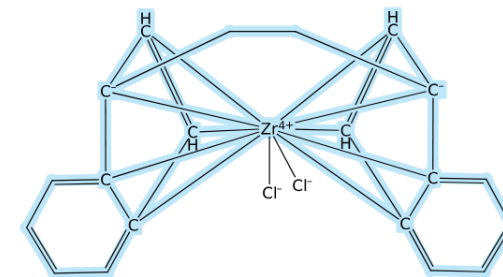
(prepn. of (2-indenyl)(1-indenyl)transition metal complexes as olefin polymn. catalysts and method of producing olefin polymer)

...

=> D FHITSTR

RN [112243-78-4](#) HCAPLUS

CN Zirconium, dichloro[1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]- (CA INDEX NAME)



Bibliographic database HCAplus

Add search precision by key words

=> S L6 AND (POLYMER? OR POLYOLEFIN or CATALYST)
L7 1022 L31 AND (POLYMER? OR POLYOLEFIN OR CATALYST)

Crossover from MARPAT

=> D BIB CLM(1)

AN 2025:340936 HCAPLUS Full-text

DN 190:40862

TI High-density ethylene-based **polymer** using hybrid supported **catalyst**,
and preparation method thereof

IN Park, Hye Ran; Kim, Sung Dong; Joung, Ui Gap; Seo, Junho; Lee, Munhee;
Kim, Ji Ho; Lim, Jae Yun; Joo, Sung Hwan

PA Hanwha Solutions Corporation, S. Korea

UO HANWHA SOLUTIONS CORPORATION

...

PI

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 2025033703	A1	20250213	WO 2024-KR9012	20240627
KR 2025022921	A	20250218	KR 2023-103175	20230807

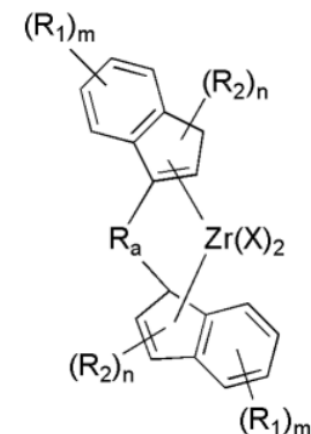
...

CLM

what is claimed is:

1. Ethylene and C under a hybrid metallocene catalyst comprising a transition metal compound of the following chemical formulas 1 to 34-C20 A method for producing high-density polyethylene by polymerizing α -olefin, wherein the hybrid metallocene catalyst is included in a molar ratio of chemical formula 1: chemical formula 2: chemical formula 3 = 1: 0.2 to 3: 1 to 7.

[Chemical Formula 1]



...

Bibliographic database HCAplus

Substance class names

=> s zirconocene and ?indenyl?
L1 1311

788 unique hits:

AN 2012:57190 HCAPLUS Full-text
DN 156:148580
TI Process for synthesizing bridged cyclopentadienyl-indenyl metallocenes
IN Yang, Qing; Hlavinka, Mark L.
PA Chevron Phillips Chemical Company LP, USA
...
PI

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 2012006268	A1	20120112	WO 2011-US42928	20110705
US 20120010421	A1	20120112	US 2010-830591	20100706
US 8309747	B2	20121113		
CN 102971334	A	20130313	CN 2011-80033371	20110705
CN 102971334	B	20151202		
EP 2590990	A1	20130515	EP 2011-738879	20110705
IN 2013DN00121	A	20140905	IN 2013-DN121	20130104

AB The present invention provides methods of making bridged cyclopentadienyl-**indenyl** metallocene compds. I (M1 = Ti, Zr, Hf; x1, x2 = F, Cl, Br, I, SO3CF3, organosulfonyl, etc.; R1R2E1 = alkylene, organosilylene, organogermylene, organostannylene, etc.; R3 = C1-18 hydrocarbyl, hydrocarbylsilyl, etc.). Generally, these methods can be conducted without the use of a fine purifn. process such as distn., chromatog., and crystn. The prepd. metallocenes are used as polymn. catalysts.

ST bridged cyclopentadienyl **indenyl** ansa metallocene prepn polymn catalyst;
ansa **zirconocene** cyclopentadienyl **indenyl** prepn polymn catalyst

Bibliographic database HCAplus

CAS LEXICON

History Project **CAS Lexicon** Databases

Metallocenes 

Clear | Collapse All

- ☐ Coordination compounds
 - ☐ Sandwich compounds
 - ☒ **Metallocenes** [Add All](#)
 - ☐ Synonyms [Add All](#)
 - ☐ Narrower Terms [Add All](#)
 - ☐ 1,1'-Bis(diphenylphosphino)ferrocene
 - ☐ Acetylferrocene [...](#)
 - ☐ Cobaltocene [...](#)
 - ☐ Nickelocene [...](#)
 - ☐ Dimethylzirconocene [...](#)
 - ☐ Ferrocene
 - ☐ Ferrocenecarboxaldehyde

History Project **CAS Lexicon** Databases

Zirconocene dichloride 

Clear | Collapse All

- ☐ Group 4 element complexes
 - ☐ Sandwich compounds
 - ☒ **Zirconocene dichloride** [Add All](#)
 - ☐ Synonyms [Add All](#)
 - ☐ Zirconocene, dichloride [...](#)
 - ☐ Zirconocene, dichloride [...](#)
 - ☐ Dichlorodicyclopentadienylzirconium
 - ☐ Dichlorodi- π -cyclopentadienylzirconium [...](#)
 - ☐ Dicyclopentadienyldichlorozirconium

History Project **CAS Lexicon** Databases

Metallocenes, Group 4 element 

Clear | Collapse All

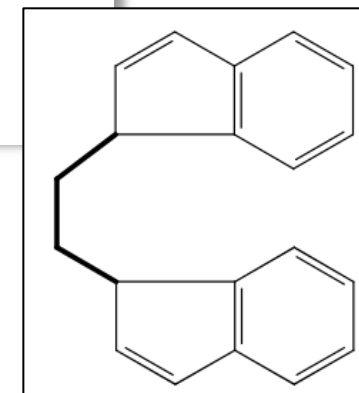
- ☐ Sandwich compounds
 - ☐ Metallocenes
 - ☒ **Metallocenes, Group 4 element metallocene complexes** [Add All](#)
 - ☐ Synonyms [Add All](#)
 - ☐ Group 4 element complexes, Group 4 element metallocene complexes [...](#)
 - ☐ Metallocene group IVB element compds. [...](#)
 - ☐ Group IVB sandwich compds. [...](#)

Consider including narrower terms, which can also include specific substances.

HCAplus - search for ligand

Search for ligand's Registry Number and refine with keywords

```
=> s 15721-07-0
L2          53 L1
=> S L2 (L) (COMPLEX OR COORDINATION OR CATALYST OR METALLOCENE)/IT AND (ZIRCON? or Zr)
L5          24 L2 (L) (COMPLEX OR COORDINATION OR CATALYST OR METALLOCENE)/IT AND (ZIRCON? OR ZR)
```



13 unique hits:

AN 2023:626860 HCAPLUS Full-text
DN 182:140723
TI Modulating comonomer selectivity using non-covalent dispersion interactions in Group 4 olefin polymerization catalysts
IN Bischof, Steven M.; Yang, Qing; Sydora, Orson L.; Lief, Graham R.; Buck, Richard M.; Ess, Daniel H.; Maley, Steven M.
PA Chevron Phillips Chemical Company LP, USA
UO CHEVRON CORP; PHILLIPS 66

...
PI

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20230098789	A1	20230330	US 2021-17403527	20210816
US 11859041	B2	20240102		
CA 3228728	A1	20230223	CA 2022-3228728	20220809
WO 2023023455	A1	20230223	WO 2022-US74676	20220809

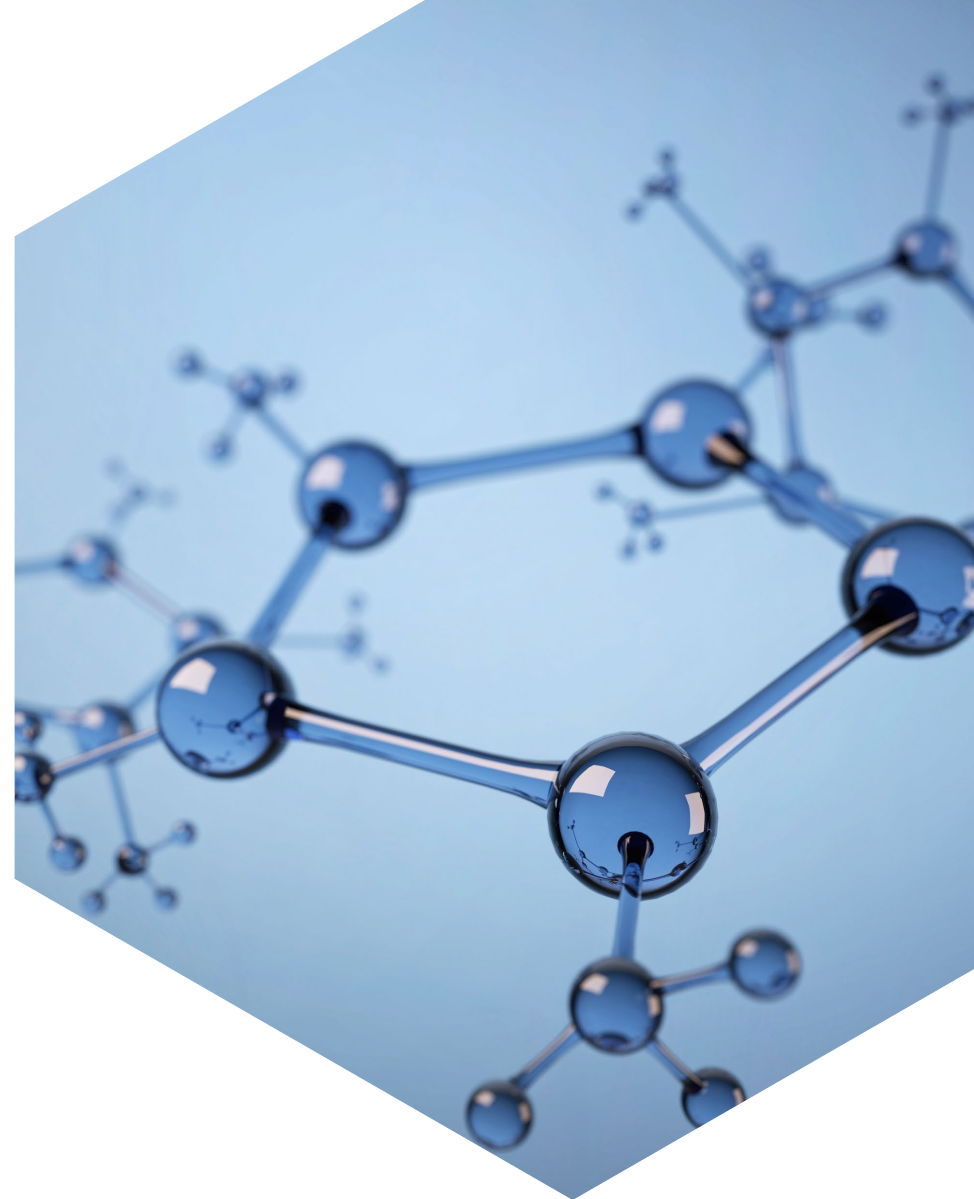
IT **15721-07-0D, zirconium complexes**
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);
PROC (Process); USES (Uses)
(modulating comonomer selectivity using non-covalent dispersion interactions in Group 4 olefin polymn. catalysts)

...

Only ligand is indexed with an appended D=Derivative!

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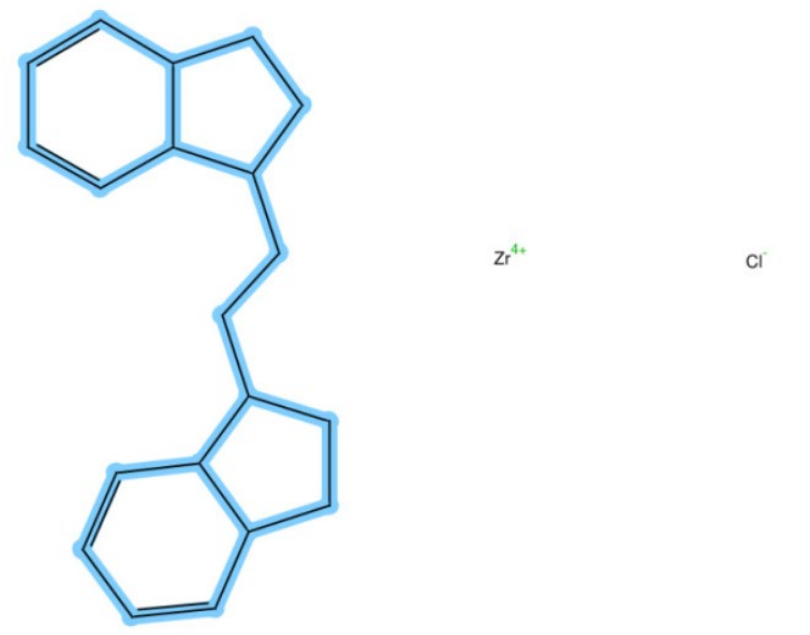
DCR records for a coordination compound

π -bonded metal

```
DCR-210988      DCR
DCSE      210988-0-0-0
CN.S      Ethylenebis(indenyl)zirconium dichloride
SY      BISINDENYLETHANEZIRCONIUM DICHLORIDE;
      ETHYLENEBIS(INDENYL)ZIRCONIUM(IV)DICHLORIDE; RAC-EN(IND)2ZRCL2;
      RAC-ETHYLENEBIS(1-INDENYL)ZIRCONIUM DICHLORIDE;
      RACEMIC-ETHYLENEBIS(INDENYL)ZIRCONIUM(IV)DICHLORIDE

CMT      1:1:2 ratio
MF      C20 H16 . Zr . 2 Cl
SMF      C20 H16 *1; Cl *2; Zr *1; TOTAL *4; TYPE *3
INCH      InChI=1S/C20H16.ClH.Zr/c1-3-7-19-15(5-1)9-11-17(19)13-14-18-12
      10-16-6-2-4-8-20(16)18;;/h1-12H,13-14H2;1H;/q;;;+4/p-1
INKY      VAEOQJQFXDXHJD-UHFFFAOYSA-M
MW      383.0235
SRIN      01391
SDCN      RA080W; RBX10E
SD      METALLOCENES
ED      Entered STN: 14 Jul 1999
      Last updated on STN: 10 Sep 2009
      Update DWPI Cross Ref.: 14 Apr 2025
```

A coordination compound with π -bonds to a π -arene ligand is usually indexed as multi-component substance ("salt") with ligand and metal as two components of the complex.

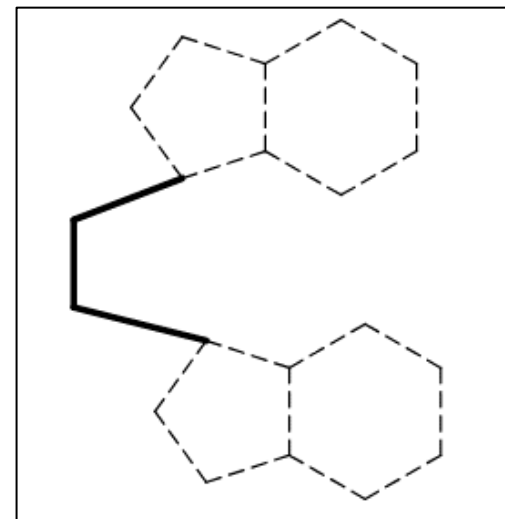


The substance descriptor field /SD can give further information on the type of substance, but is not comprehensive for searching.

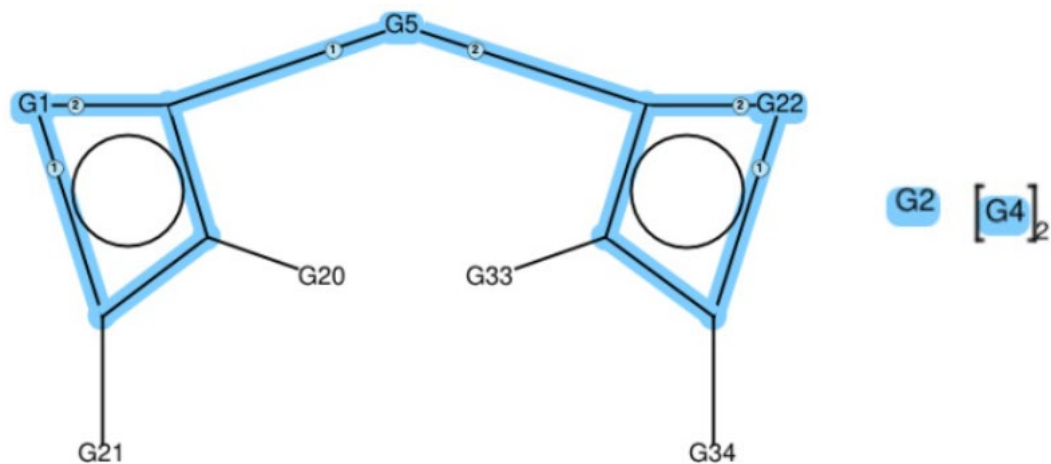
Guidelines for coordination structure queries in DCR

1. Draw ligand structure
 - Use unspecified bonds for whole ring system
 - Do not block ring fusion
 - Do not specify charges
2. Perform SSS SAMPE search, scan retrieved structures and review structure query if necessary
3. Perform SSS FULL
4. Refine with **Zr/ELS**

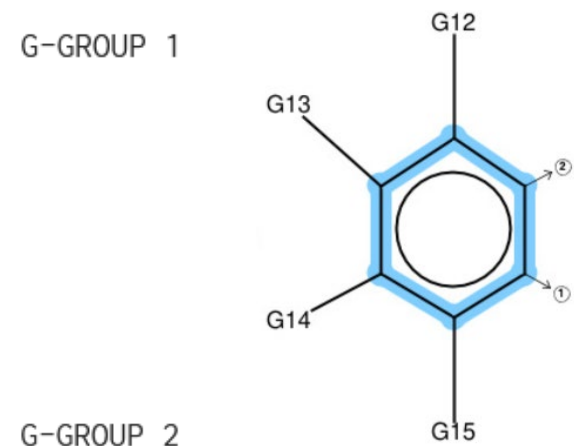
→ Search ligand and refine with **Zr/ELS**:



DWPIM record for a coordination compound



A coordination compound is indexed as the Markush structure of the ligand, where the metal is further defined in one of the G-groups.



G-GROUP 4



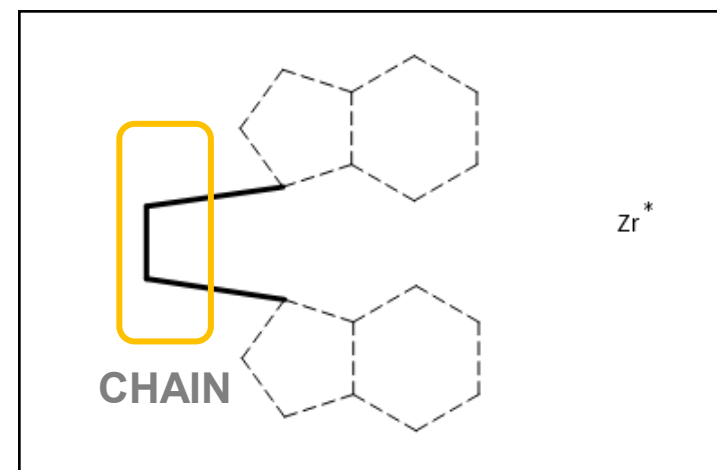
G-GROUP 5



Guidelines for coordination structure queries in DWPIM

1. Draw ligand
 - Use unspecified bonds for whole ring system
 - Assign Match level ATOM to all potentially coordinating atoms from ligand
2. Draw specific metal as separate fragment
 - Assign Match level ATOM
3. Perform SSS SAMple search,
SCAN retrieved hits, perform SSS FULL
4. View retrieved structures with **D ASB**

→ Search ligand and Zr as separate fragments:



Bibliographic database DWPI

1. Crossover DCR and DWPIM results to WPIX, refine by key words, roles or manual codes, review
2. Consider other search options in WPIX:
 - Search for different chemical names of specific compounds
 - Search for substance class name
 - Consider Manual codes to search substance classes
e.g. **A02-A06E1** - Metallocenes polymerisation catalyst containing Ti, Zr or Hf

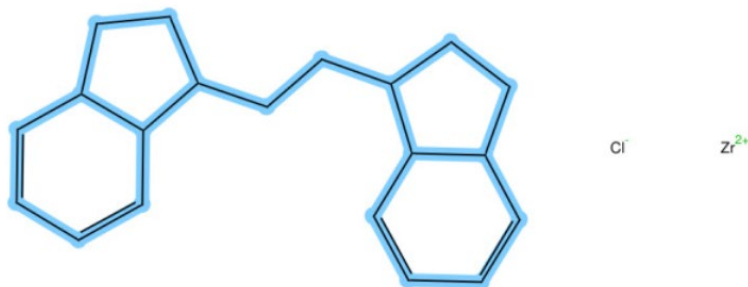
Display formats in DWPI

Crossover of results from DCR and DWPIM

=> D HITSTR

DCR hit

AN.S DCR-1941461
MF 2 Cl . C20 H16 . Zr
STR

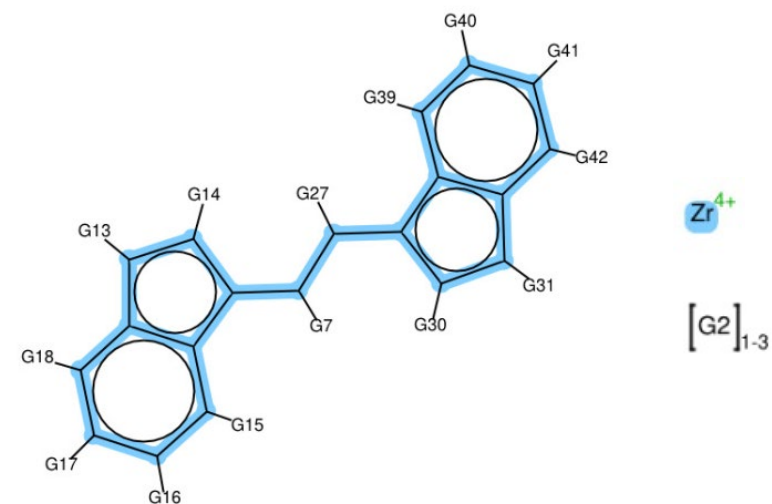


...

=> D AHITSTR

DWPIM hit

AN.M 1250-07906
SDM A : Polymers, Plastics; E : General Chemicals; C : Coordination compounds,
Complexes; Y : Mixtures
STR



...

Bibliographic database WPIX, WPIDS

Manual code searching

```
=> s A02-A06E1/MC and (Zr or zircon?) and ?indenyl?  
L2 1128
```

```
=> D FULL
```

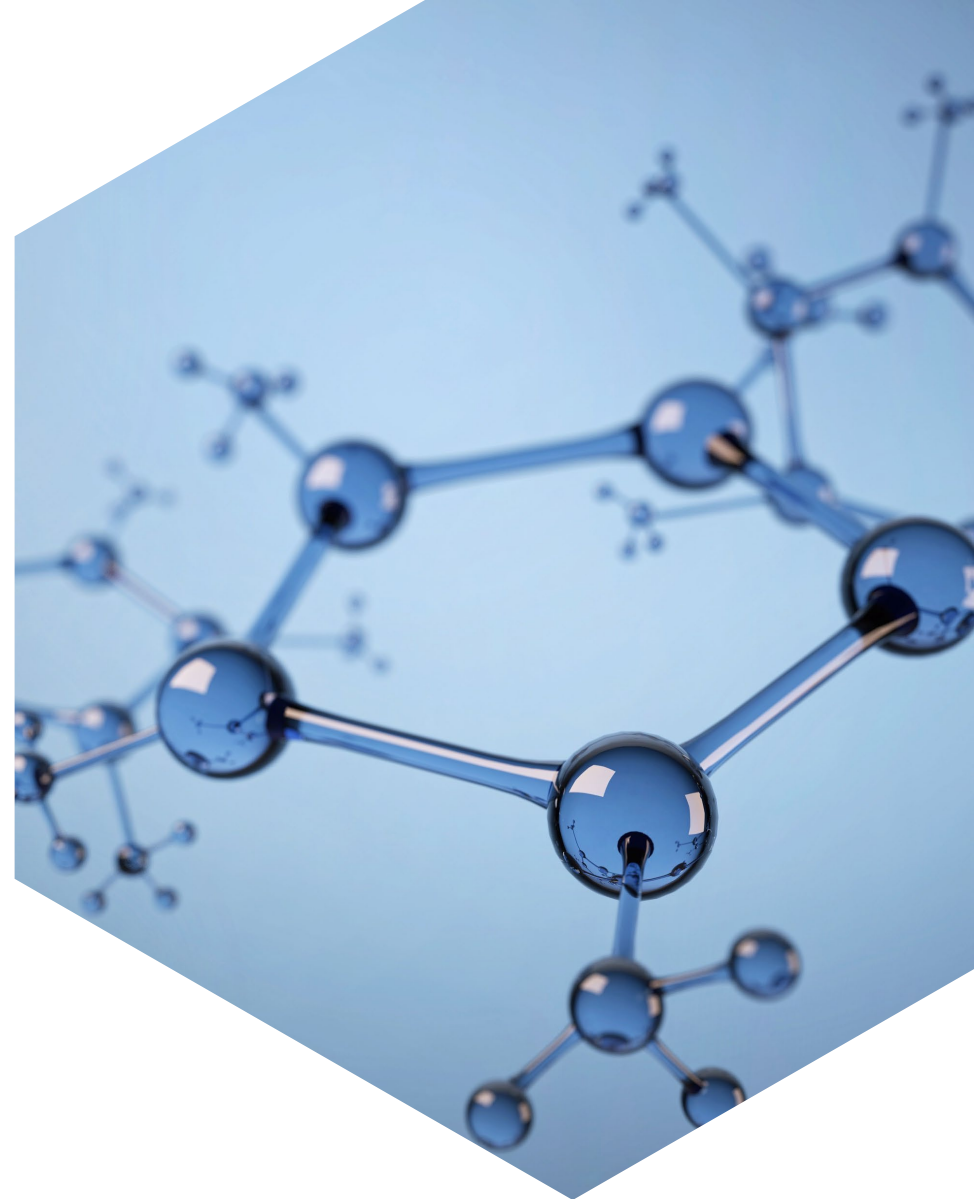
```
AN 2024-84761L [2024071] WPIX Full-text  
TI Preparation of cycloolefin copolymer used in e.g. virtual reality head  
mounted display, involves mixing norbornene and spirofluorene monomer with  
solvent, adding mixed solution, injecting ethanol acidified with  
hydrochloric acid, washing, filtering, and drying  
IN DU G; GUO S; JIN Z; WANG G  
PA (TOPO-N) TOPOLEFIN QUZHOU CO LTD  
PI CN 118420818 A 20240802 (2024071)* ZH
```

```
...  
TECH ORGANIC CHEMISTRY - Preferred Components: The solvent is n-hexane,  
cyclohexane, cyclopentane, methylcyclohexane, benzene, toluene or xylene.  
The catalyst is a metallocene, which is  
bis(cyclopentadienyl)zirconium(IV) dichloride,  
dichlorobis(indenyl)zirconium(IV).  
rac-ethylenebis-(1-η5-indenyl)-zirconium dichloride or  
rac-[1,1'-(dimethyl silylene)bis(η5-4,5,6,7-tetrahydro-1-  
indenyl)]zirconium dichloride, further comprises aluminoxane compound,  
which is methylaluminoxane or modified methylaluminoxane
```

```
...  
FS CPI; GMPI; EPI  
MC CPI: A02-A06E1; A04-B; A04-F; A04-G06A; A08-S02; A10-B04; L03-G02C;  
L03-G02G; L03-G05B7; L03-H03  
EngPI: P81-A03; P81-A09; P81-A50E1; P81-A50E5; P81-U03  
EPI: T01-J07D3A; T01-J12C; T01-J40C; U14-K01A1C; V07-F01A1; V07-F02A;  
V07-F02B; W03-A08E7A; W04-M01; W04-W07E1A
```

AGENDA

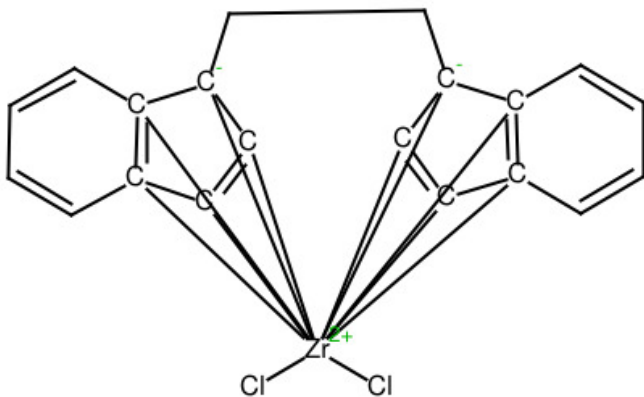
- Introduction
- Search coordination compounds:
 - In CAS files
 - In Derwent files
 - **In Elsevier files**
- Summary



ReaxysfileSUB records for a coordination compound

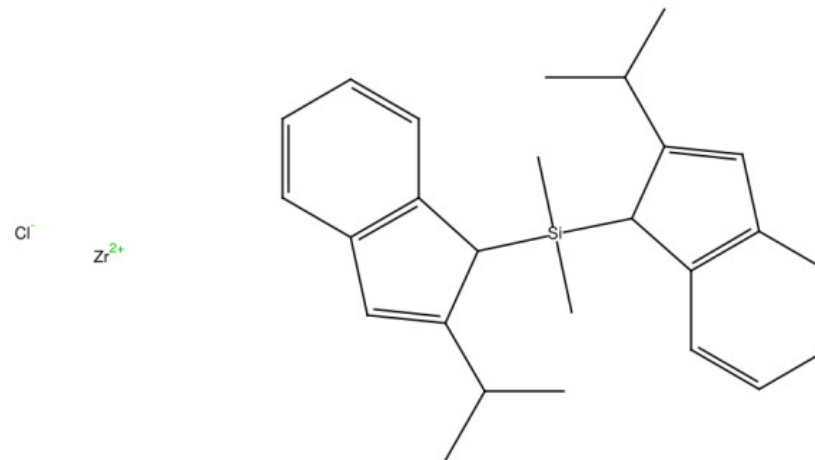
One-component substance

```
AN      11642573    REAXYSFILESU
RN      112243-78-4
CN      rac-ethanediyl-bis(1-indenyl)zirconium
dichloride; (...)
SD      coordination compound
MF      C20 H16 Cl2 Zr
CMF     C20 H16 Cl2 Zr
.
```



A coordination compound can be indexed as one-component substance...

```
AN      48887570    REAXYSFILESU
CN      bis(2-i-propyl-1-indenyl)dimethyl-silane
zirconium dichloride
MF      C26 H32 Si . 2 Cl . Zr
CMF     C26 H32 Si; 2 Cl; Zr
.
```



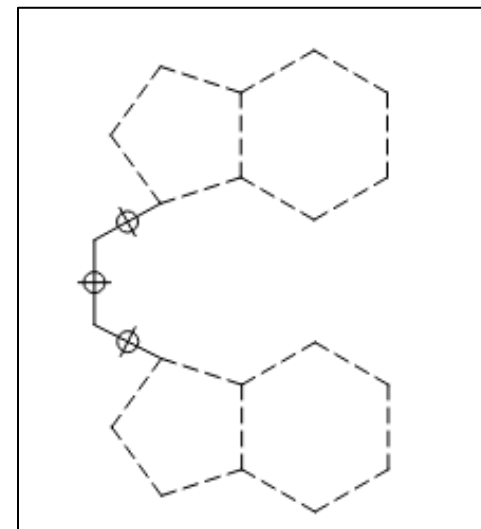
...or as multi-component substance ("salt") with ligand and metal as two components of the complex.

Note: The substance descriptor field /SD can give further information on the type of substance, but is not comprehensive for searching.

Guidelines for coordination structure queries in REAXYSFILESUB

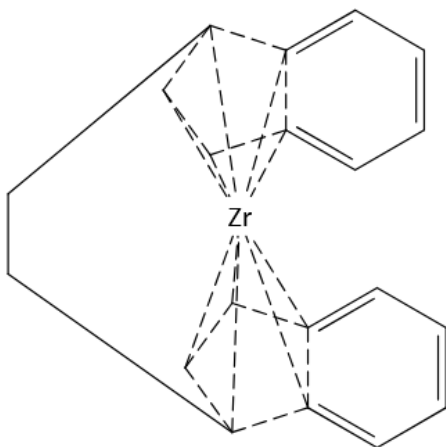
1. Draw ligand structure
 - Use unspecified bonds for whole ring system
 - Allow RING/CHAIN also for bridging bonds
 - Do not block ring fusion
 - Do not specify charges
2. Perform SSS SAMPE search, scan retrieved structures, perform SSS FULL
3. Refine with **Zr/ELS**
4. Crossover to ReaxysfileBIB, display substances with D HITSTR

→ Search ligand and refine with **Zr/ELS**:



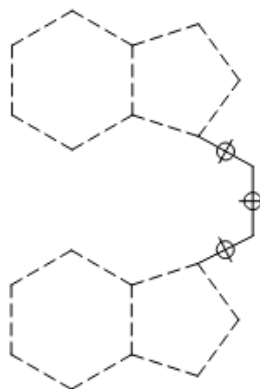
Structures to be searched

REGISTRY



DCR, REAXYFILESUB

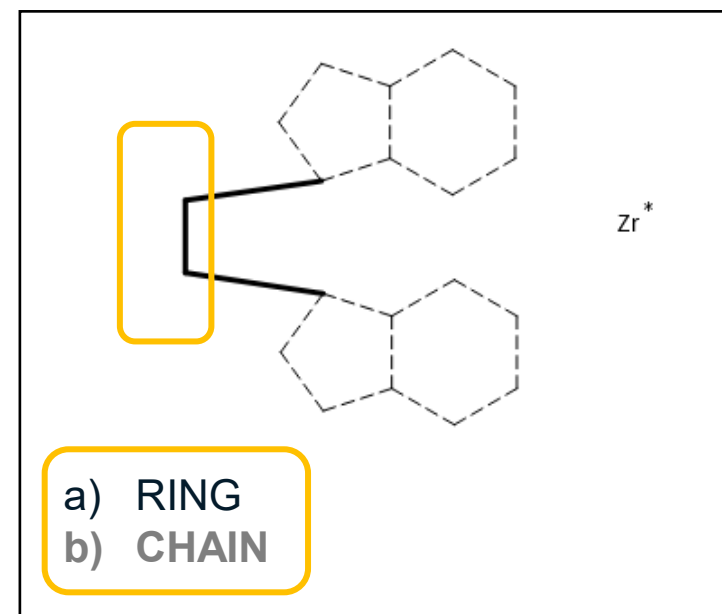
1) Search ligand structure



2) Refine with Zr/ELS

MARPAT, DWPIM

Search ligand and Zr as separate fragments



Unique hits from each database

TI Enhancing Metallocene Catalyst Activity: Utilizing Layered Double Hydroxide for Ethylene-Propylene Copolymerization

SO Macromolecular Materials and Engineering (2024), 309(1), 2300245

CAS

TI Preparation method of bimetallic active center catalyst for olefin polymerization

PI

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
CN 120484161	A	20250815	CN 2025-10566418	20250430

TI Preparing poly-alpha-olefin base oil involves catalyzing alpha-olefin monomer with metallocene catalyst-methylaluminoxane catalyst system, reacting, adding terminator, washing with water, and using alkali to separating unreacted monomer

DWPI

PI CN 113249141 A 20210813 (2021086)* ZH 10[1]
CN 113249141 B 20231226 (2024003) ZH

TI Diastereoselective synthesis of functionally substituted alkene dimers and oligomers, catalysed by chiral zirconocenes

SO Catalysis Communications (2019), volume 119, pp. 144-152

REAXYSFILEBIB

TI Polypropylene resin composition and laminate, and method for producing the same

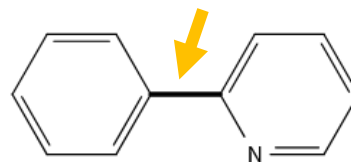
PI	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
	EP 4159439	A1	20230405		
	EP 4159439	A4	20231206		

...

Additional tips and tricks

for searching coordination compounds

- If you want to include an additional ligand or counterion:
 - Further ligands can be included in a **subset search** (or all ligands and metal drawn as fragments)
 - REG, MARPAT, DWPIM: counterions can be drawn as additional fragment in the structure editor
 - DCR, R'SUB: restrict the search to specific counterions in the field /ELS
- If substitution on coordinating rings needs to be blocked:
 - Use **non-hydrogen counts**
- Searching σ -bonded coordination compounds (e.g. NHC, Ir(ppy)₃) can be performed similarly:
 - Keep the **σ -bond unspecified**
 - Review the bond types in ligands: bridging ligand?



Summary

STNext supports **various types of coordination compound searching**

- Structure searching
- Searching reactions
- Chemical name searching
- Concept based search using value-add controlled vocabulary and classifications

For comprehensive searches utilize all search options and databases.

When searching coordination compounds be aware of indexing differences across the structure-searchable files on STNext

- Take a look at a typical example first.
- Build your structure queries accordingly.
- Use **SAM**ple structure search and **D SCAN** to quickly test your structure query.

Thank you

Larissa Bergmann
Product Specialist IP

CONTACT

Customer Center
Help@cas.org
cas.org



Comprehensive coordination compound searches

Quick guide

1) **REGISTRY:**

- Structure search for complex
- Structure search for ligand, refine by Zr/ELS
- Keyword search in /ENTE field

2) **MARPAT:**

- Structure search for ligand and metal as separate fragments in structure editor

3) **CASREACT:**

- Structure search for complex (same structure query as REG)

4) **HCAPLUS:**

- Crossover from REG, MARPAT, CASREACT
- Keyword search: chemical names, substance class names (especially for nonindexed records)
- Search for CAS RN of ligands and refine with keywords (e.g. Zircon?)

5) **DCR:**

- Structure search for ligand, refine with Zr/ELS

6) **DWPIM:**

- Structure search for ligand and metal as separate fragments in structure editor

7) **DWPI:**

- Crossover from DCR, DWPIM
- Keyword search: chemical names, substance class names
- Search for Manual codes for substance classes

8) **REAXYSFILESUB/BIB:**

- Structure search for ligand, refine with Zr/ELS
- Crossover to REAXYSFILEBIB