

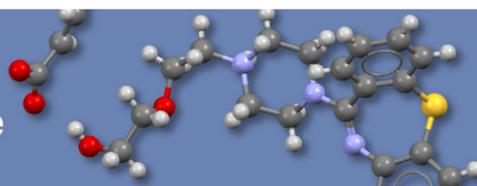
# ACCES A CAMBRIDGE STRUCTURAL DATABASE

« CSD »

## GUIDE D'UTILISATION



Celebrating 50 Years of the  
Cambridge Structural Database



CSD  
50  
1965 - 2015

## 1/Pré-requis :

- L'accès à la CSD s'effectue qu'à partir d'un poste connecté sur le réseau local de l'université.
- Firefox (dernière version).
- Java (dernière version).

## 2/ Accès à la CSD :

➔ L'accès à la CSD peut être directement accédé via l'adresse suivante :

<http://www.ccdc.cam.ac.uk/>

La page d'accueil du CSD se présente comme suit :

www.ccdc.cam.ac.uk

Rechercher

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### Celebrating 50 Years of the Cambridge Structural Database

CSD 50 1965-2015

Tweets by @ccdc\_cambridge

**Available Now!**

CSD 2016 – The world's essential database of crystal structures, over 850,000 entries  
[Introducing CSD-Enterprise](#) – ALL the data with ALL the software  
CSD-System, CSD-Discovery, CSD-Materials – New CSD-driven software suites

What's new for 2016? [Download CSD 2016](#)  
What's in the latest update? [Update CSD 2016](#)

The Cambridge Crystallographic Data Centre (CCDC) celebrates fifty years of sharing crystal structure data.  
[Find out more here.](#)

**Deposit Structures**  
Upload your data to the CCDC for inclusion in the Cambridge Structural Database

**Access Structures**  
View and retrieve structures in the Cambridge Structural Database

Structures deposited with CCDC are made publicly available for download at the point of publication or at consent from the depositor. They are also scientifically searched and included in the Cambridge Structural Database (CSD)

### 3/ Démarche :

→ Veuillez cliquer sur l'hyperlien "[Access Structures](#)" :



#### Available Now!

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**Introducing CSD-Enterprise** – ALL the data with ALL the software

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[What's in the latest update?](#)

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Upload your data to the CCDC for inclusion in the Cambridge Structural Database



#### Access Structures

View and retrieve structures in the Cambridge Structural Database

Structures deposited with CCDC are made publically available for download at the point of publication or at consent

→ Vous arriverez alors sur la page suivante :



#### Access Structures

Please use one of the following boxes to find entries in the Cambridge Structural Database.

[More information](#)

CCDC number(s)

Publication DOI or CSD DOI

CSD refcode

→ Cliquez ensuite sur le bouton « [Search Structures](#) » :



## Access Structures

Please use one of the following boxes to find entries in the [Cambridge Structural Database](#).

[More information](#)

CCDC number(s) ?

Publication DOI or CSD DOI ?

CSD refcode ?

Submit

I have none of the above

**Search Structures**

Browse Structures

[CCDC home](#)

[Deposit structures](#)

[Access structures](#)

[About this service](#)

→ Vous arriverez sur l'écran suivant :

WebCSD Entry Identifier  Family  Find Licensed to: UniversitÄfÄ© de Tlemcen at Tlemcen

[Substructure Search](#) [Similarity Search](#) [Text/Numeric Search](#) [Reduced Cell Search](#) [Browse](#) [Settings](#) [News](#) [Help](#)

WebCSD v1.0.3 Released

### WebCSD v1.1.2

The world's online portal to the Cambridge Structural Database  
Database last updated: 2016-09-28 (Updates check failed)

The main interface features a central 3D ball-and-stick model of a chlorzoxazone molecule (NEWKOP). Surrounding the model are four search options:

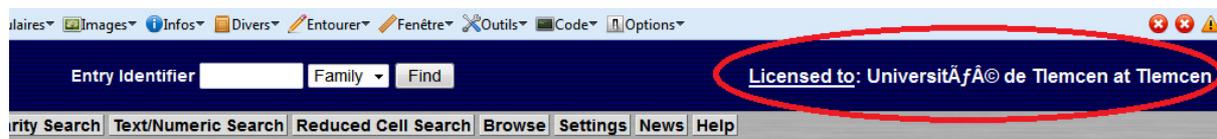
- Substructure Search**: Represented by a diagram of a substructure within a crystal lattice.
- Reduced Cell Search**: Represented by a 3D unit cell diagram with axes labeled a, b, and c.
- Similarity Search**: Represented by several chemical structures with red circles highlighting specific features.
- Text/Numeric**: Lists search criteria: Journal Reference, Bioactivity, Compound Name, Crystal Habit, CCDC Number, and All Text.

Access to WebCSD is subject to the terms and conditions of your current Licence of Access to the CSD System, site as above (top right).

Embedded visualisation in WebCSD is provided by [OpenAstexViewer](#) © 2007-2009 Mike Hartshorn and [Jmol](#) © 1998-2007 The Jmol Development Team.

Remarque :

La ligne en haut à gauche de votre écran vous permettant l'accès gratuit à la « CSD »



WebCSD v1.1.2 

The world's online portal to the Cambridge Structural Database  
Database last updated: 2016-09-28 (Updates check failed)

**Substructure Search**

**Similarity Search**

**Indexed Search**

**Text/Numeric**

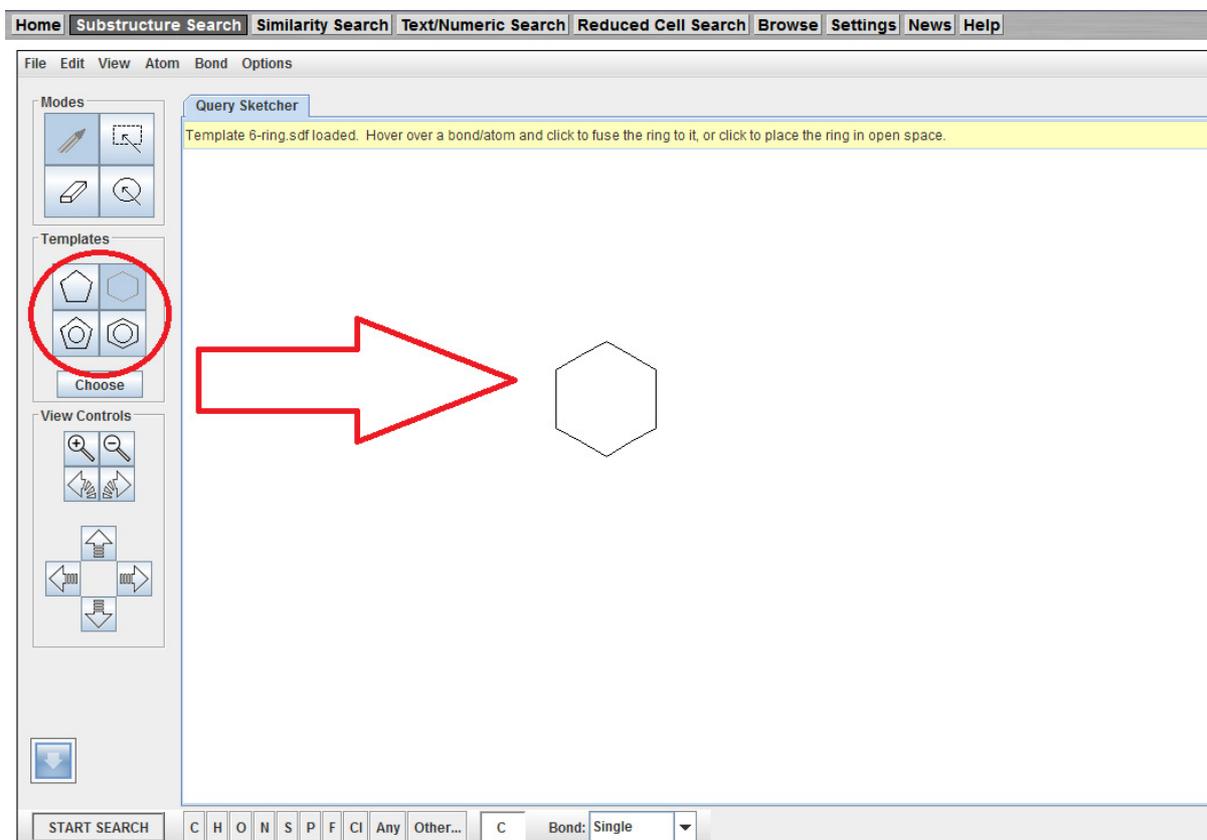
- Journal Reference
- Bioactivity
- Compound Name
- Crystal Habit
- CCDC Number
- All Text

➔ A ce stade, vous pouvez débiter la recherche

## 4/ Exemple :

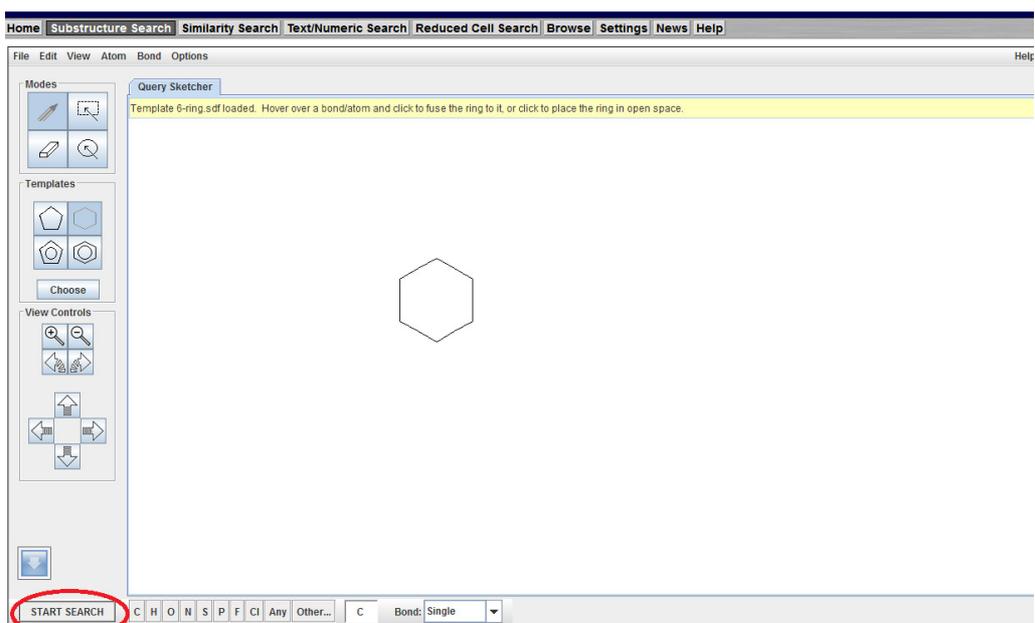
Il vous suffira ensuite de cliquer sur « **Substructure Search** » pour commencer,

➔ Choisissez la Template qui vous convient :



The screenshot shows the Query Sketcher interface. The top menu bar includes Home, Substructure Search, Similarity Search, Text/Numeric Search, Reduced Cell Search, Browse, Settings, News, and Help. The main window has a menu (File, Edit, View, Atom, Bond, Options) and a toolbar (Modes, Templates, View Controls). The Templates panel on the left shows a red circle around the hexagon template. A red arrow points from this template to a hexagon in the main workspace. The bottom status bar shows the chemical formula C H O N S P F Cl Any Other... C and Bond: Single.

➔ Cliquez ensuite sur le bouton « [START SEARCH](#) »



The screenshot shows the Query Sketcher interface after the hexagon template has been placed in the workspace. The START SEARCH button in the bottom status bar is circled in red. The chemical formula C H O N S P F Cl Any Other... C and Bond: Single are visible in the status bar.

➔ Vous arriverez sur l'écran suivant :

WebCSD Entry Identifier  Family  Find Licensed to: Université de Tlemcen at Tlemcen

Home Substructure Search Similarity Search Text/Numeric Search Reduced Cell Search Browse Settings News Help

File Filter Help

Find Entry AACMHX10

Entry	Reliability
AACMHX10	★★★★
AADAMC	★★★★
AADMPY	★★★★
AADMPY10	★★★★
AAMAND	★★★★
AANOPM	★★★★
ABACIR	★★★★
ABAFEP	★★★★
ABAFIU	★★★★
ABAGOB	★★★★
ABAHAO	★★★★
ABAPEA	★★★★
ABAOEB	★★★★
ABATRG	★★★★
ABATUT	★★★★
ABAVOO	★★★★
ABAVUU	★★★★
ABAWAB	★★★★
ABAWJ	★★★★
ABAWOP	★★★★
ABAXES	★★★★
ABAXOR	★★★★
ABAXOR01	★★★★
ABAZAE	★★★★
ABBCH	★★★★
ABRCH...	★★★★

AACMHX10 :  $\alpha$ -Acetoxy- $\alpha$ ,2-anti-diphenylmethylene-cyclohexane  
F.P.van Remoortere, J.J.Flynn; *J. Am. Chem. Soc.* (1974), **96**, 6593, doi:10.1021/ja00828a009

Hide Viewer

Diagram Details Viewer Export Options Help

View Group Symbols Key

$C_{21}H_{22}O_2$   
Space Group: P b c a  
a 24.157(6) b 16.758(4) c 8.535(2)  
 $\alpha$  90  $\beta$  90  $\gamma$  90  
R-Factor: 6.5%

➔ Vous pouvez même l'exporter sur votre pc en cliquant sur Export:

WebCSD Entry Identifier  Family  Find Licensed to: Université de Tlemcen at Tlemcen

Home Substructure Search Similarity Search Text/Numeric Search Reduced Cell Search Browse Settings News Help

File Filter Help

Find Entry AACMHX10

Entry	Reliability
AACMHX10	★★★★
AADAMC	★★★★
AADMPY	★★★★
AADMPY10	★★★★
AAMAND	★★★★
AANOPM	★★★★
ABACIR	★★★★
ABAFEP	★★★★
ABAFIU	★★★★
ABAGOB	★★★★
ABAHAO	★★★★
ABAPEA	★★★★
ABAOEB	★★★★
ABATRG	★★★★
ABATUT	★★★★
ABAVOO	★★★★
ABAVUU	★★★★
ABAWAB	★★★★
ABAWJ	★★★★
ABAWOP	★★★★
ABAXES	★★★★
ABAXOR	★★★★
ABAXOR01	★★★★
ABAZAE	★★★★
ABBCH	★★★★
ABRCH...	★★★★

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F.P.van Remoortere, J.J.Flynn; *J. Am. Chem. Soc.* (1974), **96**, 6593, doi:10.1021/ja00828a009

Hide Viewer

Diagram Details Viewer **Export** Options Help

Export

Export curated data:

File Format Crystallographic Information File (.cif) Export File

Request deposited data:

Request original deposited CIF(s) for CCDC Number 1100006  
Request all original deposited CIF(s) from this publication