

Using the CSD to augment your research

By using ConQuest

February 2021

NCS Crystallography for beginners



ConQuest features

Search for information relating to the structure determination

Structure sketcher, enabling set-up of basic substructure searches and complex 3D queries

Bibliographic search

Generic text search

Analysis of results

Elemental make-up

Show One: ConQuest – Opening and search options



ConQuest – Searching and menu options

Build Queries *Combine*

Draw

Peptide

Author/Journal

Name/Class

Elements

Formula

Space Group

Unit Cell

Z/Density

Experimental

All Text

Refcode (entry ID)

Search Reset

File Edit Options View Databases Results Help

Build Queries

Combine Queries

Manage Hitlists

View Results

View Databases Results Help

Entries in CSD version 5.41 updates

Entries in CSD version 5.41 (November 2019)

Lists in CSD version 5.41 (November 2019)

Available Databases...

CSD Pesticide subset

Best low temperature list

CSD Drug subset

CSD COVID-19 subset

Best hydrogens list

Best room temperature list

Single-component CSD Drug subset

MOF subset

ADPs available subset

Best R factor list

Non-disordered MOF subset

ConQuest – Author and journal search

Build Queries / Combine

- Draw
- Peptide
- Author/Journal**
- Name/Class
- Elements
- Formula
- Space Group
- Unit Cell
- Z/Density
- Experimental
- All Text
- Recode (entry ID)

Author/Journal (1) - Query 1

Authors' Names New Box

L.J.Mccormick Exact surname
(Required format: F.H.Allen, O'Hara, Murray-Rust etc. Brown will hit Browning unless 'Exact surname' is selected)

Journal Name

Type part of Journal name above to narrow list displayed
Select required journal in list below

- 3D Mat. [2017]
- Biotech [2015]
- J.C.A.(Spring) [1974-1975]
- A.C.S.Mtg.172,Inorg. [1976]
- AAPS PharmSciTech [2004-2013]
- ACA Abstr.Papers(Winter) [1967-1986]
- ACA,Ser.2 [1977-1984]
- ACGC Chem.Res.Comm. [2001-2009]
- ACH-Models Chem. [1994-2000]
- ACS Appl. Bio Mater. [2019]

Volume (14, 1.2 etc.) Page (212,6-A etc.) Year (1998, 2001 etc.)
during

CCDC Number (Enter numeric part only, e.g. 123456 or 123/456)

Search Store Cancel Reset

Author names should be initials followed by surname with no spaces e.g. S.J.Coles

Search Setup

Search Name: search1

Available Databases:
 CSD version 5.42 (November 2020)

You can search complete database(s) or a subset (e.g., hits found in a previous search)
Select Subset Clear Subset

Single query being used. Search will find structures:
where this query is true:
Query 1

Start Search Cancel Reset

Filters / Advanced Options

- 3D coordinates determined
- R factor <= 0.05 <= 0.075 <= 0.1
- Only Non-disordered Disordered
- No errors
- Not polymeric
- No ions
- Only Single crystal structures Powder structures
- Only Organics Organometallic

Query highlighted

Left clicking each tab will display different information

CCDC ConQuest (1) : search3 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

Refcode: AGACAP CSD version 5.42 (November 2020)

Author(s)	K.E.Thomas, K.J.Gagnon, L.J.McCormick, A.Ghosh
Reference	J.Porphyrins Phthalocyanines (2018), 22, 596
Publication DOI	10.1142/S1088424618500815
Deposition	CCDC 1534683
Formula	C ₃₇ H ₁₂ AuBr ₈ F ₁₅ N ₄ S ₃
Compound	(2,3,7,8,12,13,17,18-octabromo-5,10,15-(4'-pentafluorosulfanylphenyl)corrolato)-gold(III)
CCDC Class	Porphyrins, corrins & complexes
Spacegroup	Name: C2/c Number: 15
Cell	a: 32.932(1) b: 10.418(<1) c: 27.887(1) alpha: 90.00 beta: 96.76(<1) gamma: 90.00 Volume: 9501.419
Reduced Cell	a: 10.418 b: 17.271 c: 27.887 alpha: 96.44 beta: 90.00 gamma: 107.56 Volume: 4750.708
Molecular Volume	1187.677
Chemical Units	1
Z, Z'	Z: 8.0 Z': 1.0

AGACAP

Analyse Hitlist

- ✓ AGACAP
- ✓ AMASEO
- ✓ AMASIS
- ✓ CIMYAA
- ✓ DIJQEV
- ✓ EWEPEC
- ✓ EWEPIG
- ✓ FADJAX
- ✓ FADJEB
- ✓ FADJIF
- ✓ FADJOL
- ✓ FADJUR
- ✓ FADKAY
- ✓ FADKEC
- ✓ FEYPEH
- ✓ FEYPIL
- ✓ FEYPOR
- ✓ FIFXEA
- ✓ FIFXIE
- ✓ FIHNIV
- ✓ FIHNOB
- ✓ FIHNI IH

<< >>

120 hits

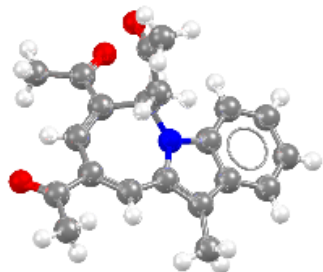
100%

Stop Search

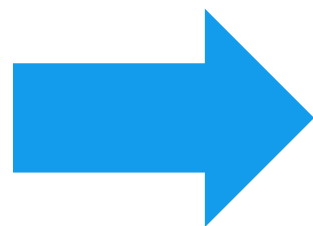
Detach

A hit list will be returned within the View Results tab of ConQuest. Left clicking on each REFCODE will toggle on and off that hit for future manipulation.

CSD Refcodes



CSD Refcode -
XOPCAJ



What is XOPCAJ?

- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

Refcode families

- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
 - Polymorphs
 - New determinations or re-refinements of the same substance
 - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc are assigned *different* refcode families

From data to publication and back

McKervey, A. R. Maguire, S. M. Tuladhar and M. Fiona Twohig, *J. Chem. Soc.* 1047–1054 DOI: [10.1039/P19900001047](https://doi.org/10.1039/P19900001047); (b) H. Duddeck, *J. Chem. Soc.*, 1055–1063 DOI: [10.1039/P19900001055](https://doi.org/10.1039/P19900001055); (c) P. Panne and J. M. Fox, *J. Appl. Cryst.* 1990, 23, 1047–1054. [External Links.](#)

ROYAL SOCIETY OF CHEMISTRY

Footnote
Electronic supplementary information (ESI) available: Experimental procedure for the synthesis of 15. For ESI and crystallographic data in CIF or other electronic format see DOI: [10.1039/C9PY00061F](https://doi.org/10.1039/C9PY00061F).

This journal is © The Royal Society of Chemistry 2009

CCDC ConQuest (1): search2 [Search]

Author(s) M. Boiocchi, M. Bonizzoni, L. Fabbrizzi, F. Foti, M. Licchelli, A. Taglietti, M. Zema

Reference [10.1039/C9PY00061F](https://doi.org/10.1039/C9PY00061F), 653

Publication DOI [10.1039/b312980b](https://doi.org/10.1039/b312980b)

CCDC 221987

Chemical formula $C_{10}H_{24}N_4Ni^{2+} \cdot 2(ClO_4^-)$

Compound (3-(4-(3-Aminopropyl)piperazin-1-yl)propylamine)-nickel(II) diperchlorate

Spacegroup Name: Pbca Number: 61

Unit cell parameters:
a: 14.426(2) b: 15.390(2) c: 16.171(2)
alpha: 90.00 beta: 90.00 gamma: 90.00
Volume: 3590.306

Reduced Cell
a: 14.426 b: 15.390 c: 16.171
alpha: 90.00 beta: 90.00 gamma: 90.00
Volume: 3590.306

Molecular Volume 448.788

Chemical Units 2

ACS Publications
Most Trusted. Most Cited. Most Read.

Polymorph α
Polymorph β

Synopsis
The pressure- and temperature-dependent transition between resorcinol polymorphs α and β has been rationalized in terms of transforming H-bonds and their networks.

Introduction
Resorcinol, an intermediate often used in chemical practice and a pharmaceutical agent, was one of the first organic compounds for which the phenomenon of polymorphism was described and the first organic compound for which the structures of both polymorphs were determined in 1938 by Robertson and Ubbelohde.^(1,2) Until today, the resorcinol crystals belong to the best known examples of polymorphs.⁽³⁾

Keywords: celecoxib; active pharmaceutical ingredient; API; solvate; crystal structure; isostructurality; disorder; PIXEL; anti-inflammatory.

CCDC references: 2011633; 2011634; 2011635; 2011636; 2011637; 2011638

Similar articles PowerPoint slides

Wiley Online Library

Two successive benzyne cycloadditions which is slightly higher than that obtained (steps). Bis-cycloadduct 15 was subjected to aromatization (TiCl₄, Zn, THF, RT, 1 h)[16] followed by hydrolysis of the silyl acetal (16) to give 17. The aromatization of 16 was carried out in a solvent mixture of CH₂Cl₂ and CH₃OH at 0 °C, 1 h, and the product was purified by column chromatography to give 17 in 73% yield.

16 M. A. Meador, H. Hart, *J. Org. Chem.* 1989, 54, 2336–2341. CrossRef | CAS | Web of Science® Times Cited: 16 | ejournals@cambridge.org - find full text'

17 CCDC 1543805 (16) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

18 Nitrile oxide 18 could be stored at -18 °C for at least one month.

Outline
Abstract
Graphical abstract
1. Introduction
2. Results and discussion
3. Conclusions
4. Experimental
Acknowledgements
Supplementary data
Research Data
References and notes

ELSEVIER SCHOLIX
Research data for this article

Cambridge Crystallographic Data Center
Crystallographic data
Data associated with the article:
CCDC 689113: Experimental Crystal Structure Determination

IUCr Journals
CRYSTALLOGRAPHY JOURNALS ONLINE

Google Scholar
Cryst. Growth Des. 12, 2147–2152. Web of Science CrossRef CAS Google Scholar
Garcia, A. (2014). *CrystEngComm*, 16, 24–27. Web of Science CSD CrossRef CAS
IUCrJ, 6, 751–760. CSD CrossRef CAS PubMed IUCr Journals Google Scholar

CCDC

CCDC ConQuest (1) : search10 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Refcode: FOPZUH

Author/Journal

Chemical Spacegroup

Crystal Name: P43212 Number: 96

Cell Parameters

a: 21.500(3) b: 21.500(3) c: 14.525(3)

alpha: 90.00 beta: 90.00 gamma: 90.00

Volume: 6714.181

Reduced Cell Parameters

a: 14.525 b: 21.500 c: 21.500

alpha: 90.00 beta: 90.00 gamma: 90.00

Volume: 6714.181

Other Parameters

Molecular Volume: 839.273 Z: 8.0

Chemical Units: 1 Z': 1.0

Additional Information

From: DMF

Habit: needle

Pol

Link to International Tables

Recrystallisation solvents and crystal shape

FOPZUH

Analyse Hitlist

- ✓ FIHPUJ
- ✓ FOPZOB
- ✓ FOPZUH
- ✓ FULLI01
- ✓ GIWFUP01
- ✓ GUPBEA
- ✓ GUPBIE
- ✓ GUPBOK
- ✓ GUPBUQ
- ✓ HAJHUW01
- ✓ HAPVEC
- ✓ JIKJAR
- ✓ KERZEP
- ✓ KIKCOY
- ✓ KOCMEX
- ✓ KOCMIB
- ✓ LAZMAD
- ✓ LAZRIQ
- ✓ LAZROW
- ✓ LAZSAJ
- ✓ LEXQIR
- ✓ NESLOR

<< >>

120 hits

100%

Stop Search

CCDC ConQuest (1) : search10 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists View Results

All Text Refcode: JIKJAR CSD version 5.41 (November 2019)

Author/Journal

Chemical Formula: $C_{48}H_{18}F_{12}N_4 \cdot 2(C_2H_4O) \cdot 0.8(H_2O)$

Crystal Name: 2,3,7,8,12,13,17,18-octaoido-5,10,15,20-tetrakis[4-(trifluoromethyl)phenyl]porphyrin methanol solvate hydrate

Chemical class

Synonym:

CCDC Class: Porphyrins, corrins & complexes

Source:

Melting Point:

Colour: red

Extra Information: Heat-sensitive, Light-sensitive, Photo-sensitive

Additional info

JIKJAR

Analyse Hitlist

- ✓ FIHPUJ
- ✓ FOPZOB
- ✓ FOPZUH
- ✓ FULLI01
- ✓ GIWFUP01
- ✓ GUPBEA
- ✓ GUPBIE
- ✓ GUPBOK
- ✓ GUPBUQ
- ✓ HAJHUW01
- ✓ HAPVEC
- ✓ JIKJAR
- ✓ KERZEP
- ✓ KIKCOY
- ✓ KOCMEX
- ✓ KOCMIB
- ✓ LAZMAD
- ✓ LAZRIQ
- ✓ LAZROW
- ✓ LAZSAJ
- ✓ LEXQIR
- ✓ NESLOR

<< >>

120 hits

100%

Stop Search

Detach

CCDC ConQuest (1) : search10 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries Manage Hitlists **View Results**

All Text
Author/Journal
Chemical
Crystal
Experimental
Diagram
3D Visualiser
CSD Internals
Search Overview

Refcode: JIKJAR CSD version 5.41 (November 2019)

Search highlighted in 2D

HO-CH₃
H₂O

Show terminal carbons

Use as Query... Detach

JIKJAR
Analyse Hitlist

- ✓ FIHPOD
- ✓ FIHPOD01
- ✓ FIHPUJ
- ✓ FOPZOB
- ✓ FOPZUH
- ✓ FULLI01
- ✓ GIWFUP01
- ✓ GUPBEA
- ✓ GUPBIE
- ✓ GUPBOK
- ✓ GUPBUQ
- ✓ HAJHUW01
- ✓ HAPVEC
- ✓ **JIKJAR**
- ✓ KERZEP
- ✓ KIKCOY
- ✓ KOCMEX
- ✓ KOCMIB
- ✓ LAZMAD
- ✓ LAZRIQ
- ✓ LAZROW
- LAZSAL

<< >>

120 hits

100%

Stop Search

Use-as-Query Options

Hydrogens:

Include hydrogen atoms

Chemical Units (molecules, ions, etc.):

Biggest chemical unit only

Make each chemical unit a separate query

Include all chemical units in a single query

Cancel OK

The screenshot shows the CCDC ConQuest (1) : search10 [Search] window. The interface includes a menu bar (File, Edit, Options, View Databases, Results, Help) and a toolbar with tabs: Build Queries, Combine Queries, Manage Hitlists, and View Results. On the left, a sidebar contains navigation options: All Text, Author/Journal, Chemical, Crystal, Experimental, Diagram, 3D Visualiser (highlighted), CSD Internals, and Search Overview. The main area displays a 3D ball-and-stick model of a complex organic molecule. Above the model, it shows 'Refcode: JIKJAR' and 'CSD version 5.41 (November 2019)'. To the right, a 'JIKJAR Analyse Hitlist' shows a list of search results with checkmarks: JIKJAR, KERZEP, KIKCOY, KOCMEX, KOCMIB, LAZMAD, LAZRIQ, LAZROW, and LAZSAJ. A context menu is open over the 3D visualiser, listing options such as Display Style (Wireframe, Capped Sticks, Ball & Stick, Spacefill), Packing, Highlight Hit, Display Hydrogens, Display Disordered Atoms, Picking Mode, Measure, Clear Measurements, Label, Settings, Save as PNG..., Save as JPEG..., Save current setting, and Reset View. A '100%' zoom level is indicated at the bottom of the menu.



Left clicking each tab will display different information



Right clicking on 3D visualiser enables you to change the display style

Packing > Molecule or unit cell

Display or hide disordered atoms

The screenshot shows the CCDC ConQuest (1) : search3 [Search] application window. The main window displays a 3D ball-and-stick model of a complex organic molecule. A 'File' menu is open, with 'Export Entries as...' selected. An 'Export Entries: search3' dialog box is overlaid on the main window. The dialog box has the following sections:

- Select file type:** A dropdown menu showing 'TAB: Tab separated list'.
- Select what to export:** Two radio buttons: 'Current entry only' (unselected) and 'All selected entries' (selected).
- Select options:** Four checkboxes: 'Bibliographic' (checked), 'Chemical' (checked), 'Crystallographic' (checked), and 'CSD internals' (unchecked).
- Either:** 'Edit Filename and Save' with a text field containing 'sers\ward\csds_data\search3.tab' and a 'Save' button.
- Or:** 'Save via' with a 'File Popup' button.
- A progress bar at the bottom shows '0%'.
- A 'Cancel' button is located to the right of the progress bar.
- A checkbox at the bottom is labeled 'Keep window open when finished' (unchecked).

You can export results in a range of different formats to save data for future manipulation.

ConQuest – Compound name search

Build Queries / **Combine**

- Draw
- Peptide
- Author/Journal
- Name/Class**
- Elements
- Formula
- Space Group
- Unit Cell
- Z/Density
- Experimental
- All Text
- Recode (entry ID)



Name/Class (1) - New

Compound Name **Contains:**

Ignore non-alphabetic characters,
e.g. "butadiene" will match "buta-1,3-diene"

Find exact word,
e.g. "hydrazine" will not match "acetylhydrazine"

Chemical Class

CCDC Chemical C...
entries in the ...
difficult to lo...
substructure or...

Note that the r...
comprehensive s...
publication tha...
specified categ...

ories of
d be

y not be
from a
he

----not defined----
Carbohydrates
Nucleosides & nucleotides
Amino-acids, peptides & complexes
Porphyrins, corrins & complexes
Steroids
Terpenes
Alkaloids
Organic polymers

Find entries classified as:

and:

ConQuest – Elements and formula search

Build Queries Combine

- Draw
- Peptide
- Author/Journal
- Name/Class
- Elements**
- Formula**
- Space Group
- Unit Cell
- Z/Density
- Experimental
- All Text
- Recode (entry ID)

Elements (1) - New

Elements Required to be Present

Type in elements, e.g. C H Se
or

Elements must be in

same molecule

same crystal structure

Other elements allowed in molecule/structure

Heaviest Permitted Element in Formula Unit

Formula (1) - New

Formula

Type in formula, e.g. C6 H12 O6
You may specify an inexact formula, e.g. Ca1-3 O>4
finds entries with 1,2 or 3 Calciums and more than 4 Oxygens.

or

Formula applies to

an individual molecule

all molecules in structure added together

Other atoms allowed in molecule/structure

Other searches

Build Queries **Combine**

- Draw
- Peptide
- Author/Journal
- Name/Class
- Elements
- Formula
- Space Group**
- Unit Cell**
- Z/Density**
- Experimental**
- All Text**
- Refcode (entry ID)

Space Group (1) - New

Enter full or partial space group symbol or number ...

... or pick from list. Click on symbol to select

- A1
- B1
- C1
- F1
- I1
- P1
- A-1

Current Space Group (with alternative settings)

Include alternative settings of selected space group

Space group and cell

Z/Density (1) - New

No. of "Molecules" per Unit Cell (Z) = []

No. of "Molecules" per Asymmetric Unit (Z')

No. of Atoms with 3D Coordinates

Calculated Density (g/cm3) = []

No. of Chemical Units (molecules, ions, etc.) in Entry

Search Store Cancel Reset

Search for cell contents

Unit Cell (1) - New

Do you want to search on the reduced cell?

You should search on reduced cell if you want to find structures which match a particular set of cell dimensions (a,b,c,alpha,beta,gamma)

Yes, do a reduced cell search No, do not do a reduced cell search

Tolerance [1.5] % of longest cell dimension

Lattice Type ----not defined----

Cell Parameters

a (A)	=	[]	alpha (°)	=	[]
b (A)	=	[]	beta (°)	=	[]
c (A)	=	[]	gamma (°)	=	[]

Search Store Cancel Reset

All Text (1) - New

Text Search | Required Fields

New Box

Either select from list or enter in box(es) below

- acicular
- air-sensitive
- bar
- black
- cream
- cube

Generic text search

The search will find words starting with what is entered in the boxes

If two or more words are typed into the same box the search will be for the exact phrase specified. To find entries containing two or more words that need not be adjacent, use the New Box button and type the required words into separate input boxes.

Search Store Cancel Reset

Experimental (1) - New

R-factor = [] fractional %

Exclude disordered structures

Exclude structures with unresolved errors

Average e.s.d. of C-C Bonds [Any]

Exclude powder structures

Temperature of Structure Determination = [] K °C

0 Room Temperature 610K

All values in the range 283-303 K are stored as Room Temperature

Irradiation Source [Any]

Search Store Cancel Reset

information on the structure determination

Storing and searching

The image shows two windows from the CCDC ConQuest software. The left window, titled 'Author/Journal (1) - Query 1', is a search form. It has a text input field containing 'L.J.McCormick' and a checkbox for 'Exact surname'. Below this is a list of journals, with '2D Mat. [2017]' selected. At the bottom, there are fields for 'Volume', 'Page', and 'Year', and a 'CCDC Number' field. The 'Store' button is highlighted in blue. A blue arrow points from this button to the right window.

The right window, titled 'CCDC ConQuest (1) : search1 [Search]', shows the search results. It has a menu bar with 'File', 'Edit', 'Options', 'View Databases', 'Results', and 'Help'. Below the menu are tabs for 'Build Queries', 'Combine Queries', 'Manage Hitlists', and 'View Results'. On the left is a vertical list of search criteria: Draw, Peptide, Author/Journal, Name/Class, Elements, Formula, Space Group, Unit Cell, Z/Density, Experimental, All Text, and Refcode (entry ID). The 'Author/Journal' criterion is selected. The main area shows two query entries: 'Query 1' (checked) for 'Author L.J.McCormick' and 'Query 2' (checked) for a chemical structure. The chemical structure is a complex organic molecule with trifluoromethyl groups and a central ring system. Below the structure is the text 'From JIKJAR' and a '2D' label. At the bottom of the window are 'Search' and 'Reset' buttons.

Combining queries and managing hitlists

CCDC ConQuest (1) : search1 [Search]

File Edit Options View Databases Results Help

Build Queries **Combine Queries** Manage Hitlists View Results

Drag Query Icons into Boxes

Find entries that:

must have (boolean AND)

Query 1

must not have (NOT)

Query 2

must have at least one of (OR)

Search Reset

Query 1 Author L.J.McCormick Edit... Delete

Query 2 Edit... Delete

Chemical structure diagram showing a complex organic molecule with fluorine and nitrogen atoms. From JIKJAR

CCDC ConQuest (1) : search2 [Search]

File Edit Options View Databases Results Help

Build Queries Combine Queries **Manage Hitlists** View Results

Combine Hitlists

Combination Name: combination1

List A search1 List B search2

Include deselected entries in:

List A List B

Generate a List of Entries:

common to List A and List B

in either List A or List B

in List A but not in List B

OK

Hitlist Overview

search1 (120 Entries)

Author L.J.McCormick

Name	Hits	Type
search1	120	Search
search2	1	Search

Delete Rename... Notes... View

Tip - You can rename a search

Draw

Build Queries **Combine**

- Draw
- Peptide
- Author/Journal
- Name/Class
- Elements
- Formula
- Space Group
- Unit Cell
- Z/Density
- Experimental
- All Text
- Refcode (entry ID)

The screenshot shows the 'Draw (1) - New' window with a menu bar (File, Edit, Atoms, Bonds, 3D, Options, Help) and a toolbar. The 'Atoms' menu is open, showing options like 'Element', 'Add Group', 'Expand Chemical Groups', 'Hydrogens', 'Charge', 'Number of Bonded Atoms', 'Cyclic', and 'All Atoms in Same Molecule'. The 'Options' menu is also open, showing 'Drawing Options...', 'Snap to Grid', 'Save Window Size', 'Limit Window Size', 'Auto-Generate H', and 'Balloon Help'. The 'DRAW' button in the toolbar is highlighted. The '3D Parameters' panel on the right shows 'Next Atom: C' and 'Next Bond: Single'. The 'Contacts' panel is also visible. The bottom toolbar contains buttons for 'C', 'H', 'O', 'N', 'S', 'P', 'F', 'Cl', 'Any', 'More...', 'Groups...', and a 'Bond' dropdown set to 'Single'.

Additional menu options to explore

Define atoms, bonds or molecules to be searched

Define lengths, angles, torsions or geometric objects e.g. plans or centroids as parameters to be searched

Ring template selector or builder

List of templates for challenging structures e.g. adamantane

Select specific or general atom types/functional groups

Select bond type

ConQuest – Draw/Structure search

Build Queries Combine

Draw

Peptide

Author/Journal

Name/Class

Elements

Formula

Space Group

Unit Cell

Z/Density

Experimental

All Text

Recode (entry ID)

Draw (1) - New

File Edit Atoms Bonds 3D Options Help

Click and drag to create a bond.
Drag to an existing atom to make a connection.

Next Atom: C
Next Bond: Single

3D Parameters:

Options...
Delete

Contacts:

Options...
Delete

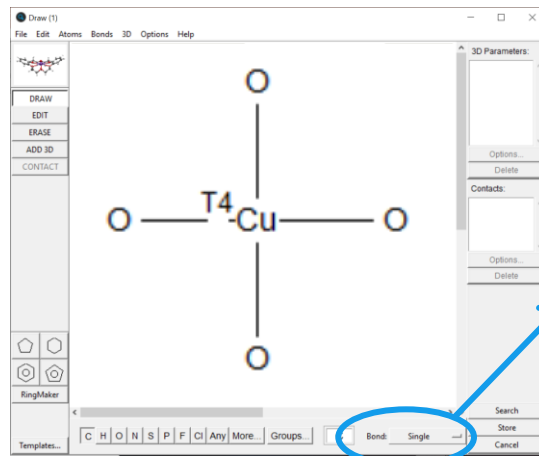
Search
Store
Cancel

O=C-C-7A

Templates... C H O N S P F Cl Any More... Groups... C Bond: Single

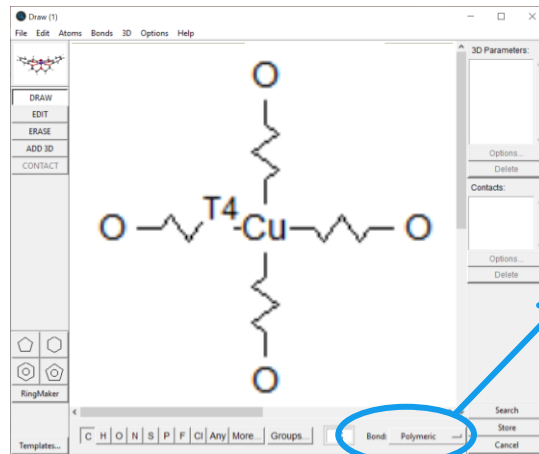
Example of a search, where 7A represents any halogen

Substructure found



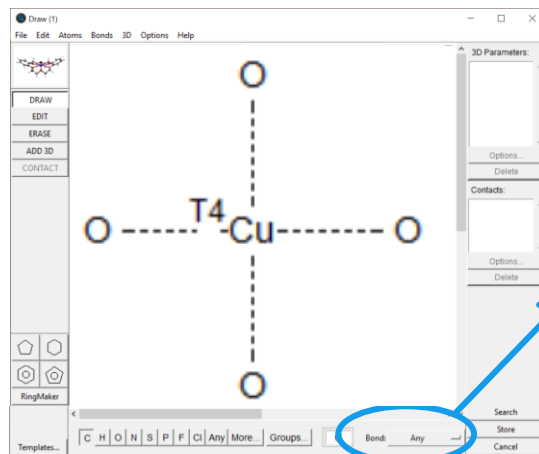
Bond:

- Single
- Double
- Triple
- Quadruple
- Aromatic
- Polymeric
- Delocalised
- Pi
- Any
- Variable...



Bond:

- Single
- Double
- Triple
- Quadruple
- Aromatic
- Polymeric
- Delocalised
- Pi
- Any
- Variable...



Bond:

- Single
- Double
- Triple
- Quadruple
- Aromatic
- Polymeric
- Delocalised
- Pi
- Any
- Variable...

Using "Any" bond can help find more complicated structures such as polymers, delocalised and pi-bonded systems

