

DEPARTAMENTO DE QUÍMICA INORGÁNICA

Tutorial sobre los recursos docentes del [Cambridge Crystallographic Data Centre](http://www.ccdc.cam.ac.uk)
<http://www.ccdc.cam.ac.uk>

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El **Cambridge Crystallographic Data Centre** (CCDC) es una institución sin ánimo de lucro surgida en la Universidad de Cambridge (Reino Unido), cuya misión principal es la recolección y preservación de datos estructurales de sustancias químicas para su posterior aplicación en investigación, principalmente para el descubrimiento de nuevos fármacos y el desarrollo de materiales. El CCDC gestiona y mantiene la **Cambridge Structural Database** (CSD), una base de datos de estructuras moleculares determinadas experimentalmente mediante difracción de rayos X de monocristal, la cual se ha convertido en el principal repositorio de estructuras de compuestos orgánicos y complejos organometálicos y de coordinación.

El CCDC está profundamente comprometido con el uso de estos datos en educación. Para ello, han promovido la creación de materiales educativos que utilizan las estructuras cristalinas depositadas. En la página <https://www.ccdc.cam.ac.uk/Community/educationalresources/>, se recopila toda la actividad de este centro relacionada con la educación.

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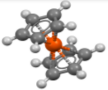
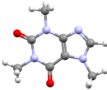
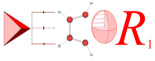






Training and Educational Resources

The wealth of information contained within the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials informs much of chemistry, biochemistry, and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore.

The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of course, our database of over one million entries are available for free through our Access Structures portal.

If you are an educator looking for supplementary teaching materials, find out more about the Teaching Database [here](#). If you have developed your own modules using the CSD and would like to share them with the broader community, please contact us at education@ccdc.cam.ac.uk.

To keep up to date with the latest news from education and outreach at the CCDC, sign up for the Education and Outreach Newsletter [here](#).

-  Information on the Teaching Subset
-  Access a series of teaching modules for use in the classroom
-  DECOR: Educational Resources for Teaching Crystallography
-  Download a series of self-guided workshop materials for CCDC tools and features
-  Watch software training and support videos
-  CSDU modules - Explore our on-demand training courses
-  Access fun science activities for kids through the CCDC Home learning page
-  Explore the Periodic Table through Crystal Structures
-  Bound! a Protein-Drug matching card game

1. Teaching subset

El **Teaching Subset** es un subconjunto de estructuras cristalinas de la CSD que ha sido seleccionado para ser utilizado en docencia. En la página web <https://www.ccdc.cam.ac.uk/Community/educationalresources/teaching-database/> se encuentra toda la información sobre cómo acceder y algunos ejemplos de aplicación.

Mediante el siguiente enlace, <https://www.ccdc.cam.ac.uk/structures/search?compound=Teaching%20Subset>, se accede al subconjunto completo, que contiene más de 750 estructuras, clasificadas en **Fundamental Chemistry**, **Drug Molecules**, **Symmetry**, **MOFs** y **Essential Nutrients**.

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Teaching Subset

Our 750+ structure teaching subset includes a wide variety of molecules (from adrenaline to zirconium complexes) and can be used to enhance learning across the chemistry curriculum. A range of associated teaching units demonstrate how the interactive on-line teaching database can be used to teach core chemistry concepts.

What is in the Teaching Subset

Entries in the teaching subset have been classified by the various concepts they are used to demonstrate. Click on the header for each classification to view the structures included.



Fundamental Chemistry

These entries serve to demonstrate fundamental chemistry concepts such as VSEPR theory, coordination chemistry, geometry, chirality and isomerism. They may also contain examples of common classes of organic compounds or functional groups such as alkanes, alkenes, alkynes, ketones, esters, acids, alcohols and aldehydes. Entries may also include common molecules of interest such as cholesterol, caffeine, or fullerene.

Por ejemplo, en **Fundamental Chemistry**, podemos encontrar un listado de estructuras disponibles.

The screenshot shows the CCDC Access Structures interface. At the top, there are search tabs: Simple Search, Structure Search, Unit Cell Search, and Formula Search. Below the search bar, it indicates the query: "Your query was: Compound name: Teaching Subset and the search returned more than 30 records." There are buttons for "Modify Search" and "New Search". Below this, there are buttons for "Select all", "Download Selected", and "View Selected". The main content area displays a list of search results for "Fundamental Chemistry". Each result includes a checkbox, a chemical structure image, and detailed information:

- ABABEL**: Deposition Number(s): 243822, Teaching Structure, Space Group: P 2₁/c (14), Cell: a 11.1366(12)Å b 6.9872(7)Å c 15.3869(16)Å, α 90° β 93.796(2)° γ 90°, Compound Name: 4-Chloro-3-phenylquinolin-2(1H)-one, Synonyms: Teaching Subset; Fundamental Chemistry.
- ABAFUF**: Deposition Number(s): 243848, Teaching Structure, Space Group: P c (7), Cell: a 14.8129(3)Å b 9.52300(20)Å c 14.1217(3)Å, α 90° β 105.076(1)° γ 90°, Compound Name: (R,R)-Dichloro-(N,N'-dibenzyl-N,N'-dimethylethylenediamine)-palladium(II), Synonyms: Teaching Subset; Fundamental Chemistry, Symmetry.
- ABALEV**: Deposition Number(s): 244176, Teaching Structure, Space Group: P 2₁ (4), Cell: a 10.692(2)Å b 8.858(2)Å c 11.968(2)Å, α 90° β 114.40(1)° γ 90°, Compound Name: (1S,3S)-1,3-bis(4-Bromophenyl)-2-methylpropane-1,3-diol isopropanol solvate, Synonyms: Teaching Subset; Fundamental Chemistry.
- ABCLUA10**: Deposition Number(s): 1100072, Teaching Structure, Space Group: P 2₁ (4), Cell: a 11.206(6)Å b 8.248(4)Å c 14.272(7)Å, α 90° β 107.66(2)° γ 90°, Compound Name: 5,9-Diacetyl-(3,6)bicycloleuconolide A₃, Synonyms: Teaching Subset; Fundamental Chemistry.

Estas estructuras pueden explorarse directamente en la web pulsando sobre el identificador. Se abre una nueva página, con toda la información sobre la estructura y un visualizador 3D con varias opciones de representación y muchas funciones:

CCDC FIZ Karlsruhe Leibniz Institute for Information Infrastructure CSD Entry: ABAFUF Pablo Gonzalez-Herrero

Simple Search Structure Search Unit Cell Search Formula Search

Your query was: Compound name: Teaching Subset and the search returned more than 30 records.

Back to Search List Modify Search New Search

Database Identifier	Deposition Number
ABAFUF	243848

Next Download

ABAFUF : (R,R)-Dichloro-(N,N'-dibenzyl-N,N'-dimethylethylenediamine)-palladium(II)
Space Group: P c (7), Cell: a 14.8129(3)Å b 9.52300(20)Å c 14.1217(3)Å, α 90° β 105.076(1)° γ 90°

3D viewer
Ball and Stick No Labels

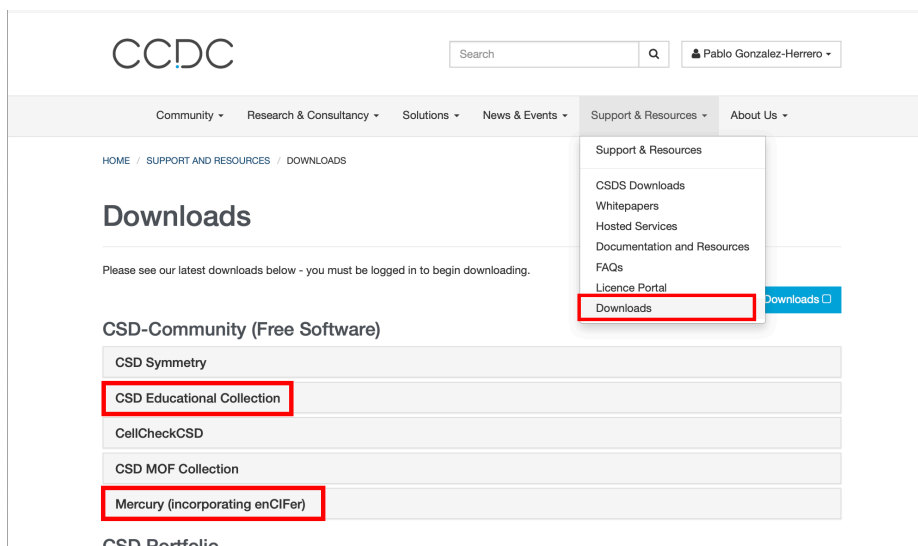
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Chemical diagram

CN(C)CCN(C)C1=CC=C(C=C1)C1=CC=C(C=C1)Cl[Pd]Cl1=CC=C(C=C1)C1=CC=C(C=C1)C

También se pueden descargar todas las estructuras de este subconjunto en formato CIF en la página de descargas del CCDC. Para ello, es necesario registrarse como usuario.

Otra forma de acceder es mediante el programa **Mercury**, que también se puede descargar gratuitamente desde la página de descargas del CCDC. Este programa permite abrir archivos CIF y otros formatos de estructuras moleculares para visualizarlas en 3D. Mediante el menú **CSD-Community** se accede al Teaching Subset seleccionando **Open Teaching Database**.



2. Módulos para docencia (*Teaching Modules*)

El CCDC ha recopilado una serie de módulos para docencia que pueden utilizarse en diferentes niveles educativos, desde la educación secundaria hasta la universitaria. Pueden descargarse directamente en formato PDF desde la web: <https://www.ccdc.cam.ac.uk/Community/educationalresources/teaching-modules/>

Los más interesantes para la docencia universitaria son los siguientes:

- Introduction to optical isomerism and chirality
- Introduction to Symmetry Operations and Point Groups
- Learning Point Group symmetry through 3D printed models
- Metal-Organic Concepts
- Hydrogen-Bonding Concepts

3. Recursos adicionales

Existe un blog creado por educadores que utilizan la CDS, al que se puede acceder mediante el enlace: <https://www.ccdc.cam.ac.uk/Community/blog/tags/CSD%20Educators>

También se ha recopilado una lista de reproducción de vídeos de **YouTube** en los que se muestra cómo los educadores usan el Teaching Subset y el software de la CSD. Se accede en: <https://www.youtube.com/playlist?list=PLEtBZ08SGISfgA8EupmwC0TF74ZOJhrPA>