‘***Cambridge Structural Database (CSD)***’

Στη βάση δεδομένων ‘***Cambridge Structural Database (CSD)***’ του ***Cambridge Crystallographic Data Centre (CCDC)*** [http://www.ccdc.cam.ac.uk/] έχουν αρχειοθετηθεί πάνω από 500.000 κρυσταλλικές δομές μικρών μορίων. Η τεράστια ανάπτυξη της CSD βάσης δεδομένων, τόσο ως προς το πλήθος, όσο και ως προς την πολυπλοκότητα των κατατιθέμενων δομών, όχι μόνο δίνει σημαντικές απαντήσεις για τις μοριακές δομές και τις αλληλεπιδράσεις τους αλλά και βοηθά στη σωστή κατεύθυνση της έρευνας για την κατανόησή τους.

History of Crystallography and the Cambridge Structural Database

The development of X-ray crystallography has been rapid, and since the diffraction of X-rays by crystals was discovered by von Laue in 1912 the technique has attracted 24 Nobel Prizes. Indeed, crystal structure analysis is now central to modern chemistry - it is the method of choice for the characterisation of newly discovered compounds - and it is distinguished from other analytical methods by the sheer richness of the information that it provides: not only does it give the precise three-dimensional structure and geometry of individual molecules, but also vital information about how molecules interact with each other. In the words of Professor Chet Raymo in the Boston Globe, *"Crystals are windows on the world of atoms"*.

While individual determinations of organics and metal-organics have value, taken collectively crystal structures provide knowledge that transcends individual results and is key to our understanding of chemical and biological processes. For this reason a high quality, fully curated database is a unique scientific resource. The CCDC began operations in 1965 with a brief to build the Cambridge Structural Database (CSD) - the worldwide repository of carbon-containing small-molecule crystal structures. One of the world's first numerical database systems, compilation of the CSD began with just a few hundred structures.

Today, the CCDC archives approximately 150 new experimentally determined structures each working day. Each structure is fully checked and validated by expert chemists and crystallographers, and entries are further enriched with valuable chemical data. As the world's output of crystal structures continues to accelerate, the CSD has doubled in size in the last 9 years and now contains a fully retrospective collection of half a million entries. Notable examples include the structures of amino-acids, steroids, alkaloids, antibiotics including penicillin, ferrocenes, fullerenes, catalysts, etc. Within this massive structural diversity, normal molecules are abundant and unusual molecules are commonplace.

The Cambridge Structural Database - The world repository of small molecule crystal structures

The Cambridge Structural Database (CSD) is the principal product of the CCDC. It is the central focus of the CSD System, which also comprises software for database access, structure visualisation and data analysis, and structural knowledge bases derived from the CSD.

The CSD records bibliographic, chemical and crystallographic information for:

- organic molecules
- metal-organic compounds

whose 3D structures have been determined using

- X-ray diffraction
- neutron diffraction

The CSD records results of:

- single crystal studies
- powder diffraction studies

which yield 3D atomic coordinate data for at least all non-H atoms. In some cases the CCDC is unable to obtain coordinates, and incomplete entries are archived to the CSD.

The CSD includes crystal structure data arising from:

- publications in the open literature
- Private Communications to the CSD (via direct data deposition)

The CSD does not store:

- Polypeptides and polysaccharides having more than 24 units. These are recorded in the Protein Data Bank http://www.rcsb.org/pdb/
- Oligonucleotides. These are stored in the Nucleic Acids Data Bank http://ndbserver.rutgers.edu/
- Inorganic structures, which are stored in the Inorganic Crystal Structure Database http://www.fiz-karlsruhe.de/icsd_content.html
- Metals and Alloys, which are stored in CRYSTMET® http://www.tothcanada.com/

Cambridge Crystallographic Data Centre (CCDC)
→ Free Services → Request a Structure
http://www.ccdc.cam.ac.uk/products/csd/request/

Το αρκτικόλεξο CIF (*Crystallographic Information File)*
Τυποποιημένη μορφή (format) αρχείου από τους Hall, Allen & Brown (1991) για την ανταλλαγή κρυσταλλογραφικών δεδομένων

- The Crystallographic Information File (CIF): a New Standard Archive File for Crystallography, S. R. Hall, F. H. Allen and I. D. Brown.
  Acta Cryst. (1991). **A47**, 655-685.

ΠΑΡΑΔΕΙΓΜΑ:

Carbohydrate Research 344 (2009) 2606–2608

Contents lists available at ScienceDirect

Carbohydrate Research

journal homepage: www.elsevier.com/locate/carres

Note

An investigation of the inclusion complex of cyclomaltoheptaose (β-cyclodextrin) with *N*-methylanthranilic acid in the solid state

N. R. Lien [a], J. R. Telford [b,*]

[a] Department of Chemistry, Whitman College, Walla Walla, WA 99362, USA
[b] College of Liberal Arts and Sciences, Maryville University, St. Louis, MO 63141, USA

ARTICLE INFO

Article history:
Received 12 June 2009
Received in revised form 14 September 2009
Accepted 16 September 2009
Available online 19 September 2009

Keywords:
Supramolecular chemistry
Cyclomaltoheptaose
β-Cyclodextrin
Crystal structure
Inclusion complex

ABSTRACT

A 2:1 complex between cyclomaltoheptaose (β-cyclodextrin) and *N*-methylanthranilic acid has been studied in the solid state. The inclusion complex belongs to the triclinic system (space group *P*1) with unit cell dimensions $a = 15.2773(15)$ Å, $b = 15.4710(15)$ Å, $c = 17.9627(18)$ Å, $\alpha = 99.632(5)°$, $\beta = 113.416(5)°$, and $\gamma = 102.818(5)°$. The complex forms a head-to-head channel-type structure with the *N*-methylanthranilic acid lying between the β-cyclodextrin groups in a sandwich fashion, which is held in place by an extensive hydrogen-bonding network between the cyclodextrin molecules.

...

2. Supplementary data

Complete crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC no. 735463. Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK. (fax: +44 1223 336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk).

CIF

Chemical info

…

```
_chemical_name_common            'Cyclodextrin and N-methyl
Anthranilic Acid'
_chemical_melting_point          ?
_chemical_formula_moiety         ?
_chemical_formula_sum            'C102.05 H142 N O99.94'
_chemical_formula_weight         2981.83
```

…

Crystallographic info

```
loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'

_cell_length_a                   15.2773(15)
_cell_length_b                   15.4710(15)
_cell_length_c                   17.9627(18)
_cell_angle_alpha                99.632(5)
_cell_angle_beta                 113.416(5)
_cell_angle_gamma                102.818(5)
_cell_volume                     3640.7(6)
_cell_formula_units_Z            1
_cell_measurement_temperature    190(2)
_cell_measurement_reflns_used    ?
_cell_measurement_theta_min      2.91
_cell_measurement_theta_max      27.48
```

…

Structural info

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_calc_flag
...
C8 C 0.8804(14) 0.7048(17) 0.6710(15) 0.092(10) Uani 0.53(5) 1 d PD .
O2 O 0.748(4) 0.920(5) 0.660(7) 0.82(14) Uiso 1.00(18) 1 d D . .
```

…

```
loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
C8 0.084(14) 0.113(18) 0.112(18) 0.074(14) 0.042(12) 0.066(13)
O81 0.038(2) 0.061(3) 0.049(3) 0.028(2) 0.008(2) 0.002(2)
```

…

_geom_special_details

…