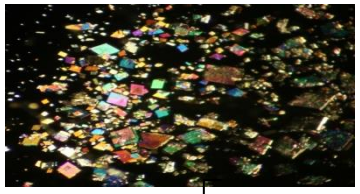
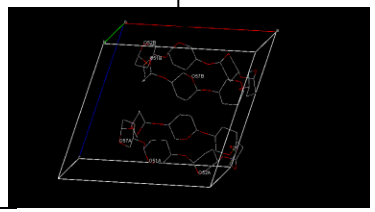
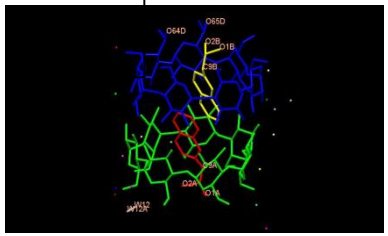
ΔΙΑΓΡΑΜΜΑ ΡΟΗΣ



Σύστημα κρυσταλλογραφίας Εργαστηρίου Φυσικής ΓΠΑ





ΚΑΤΑΣΚΕΥΗ ΚΡΥΣΤΑΛΛΟΥ

ΣΥΛΛΟΓΗ ΠΕΙΡΑΜΑΤΙΚΩΝ ΔΕΔΟΜΕΝΩΝ ΑΠΟ

ΠΕΡΙΘΛΑΣΗ ΑΚΤΙΝΩΝ Χ

ΠΕΙΡΑΜΑΤΙΚΕΣ Ή ΑΜΕΣΕΣ ΜΕΘΟΔΟΙ ΠΡΟΣΔΙΟΡΙΣΜΟΥ ΑΡΧΙΚΟΥ ΣΥΝΟΛΟΥ ΦΑΣΕΩΝ

ΑΡΧΙΚΟ ΠΡΟΤΥΠΟ

ΒΕΛΤΙΣΤΟΠΟΙΗΣΗ

ΣΥΜΠΛΗΡΩΣΗ ΠΡΟΤΥΠΟΥ

ΑΞΙΟΛΟΓΗΣΗ

ΑΠΟΘΗΚΕΥΣΗ ΔΕΔΟΜΕΝΩΝ (ΑΡΧΕΙΑ ΜΟΡΦΗΣ .CIF, .PDB, κα)

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 characterization of newly discovered compounds - and it is distinguished from other analytical methods by the sheer richness of the information that it provides:

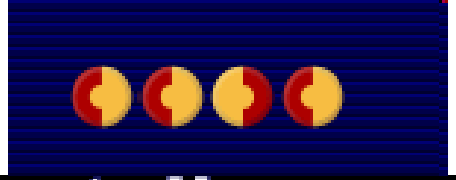
not only does it give the precise three-dimensional structure and geometry of individual molecules, but also vital information about how molecules interact with each other.

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.



Cambridge Crystallographic Data Centre

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

Στη βάση δεδομένων '***Cambridge Structural Database (CSD)***' του ***Cambridge Crystallographic Data Centre (CCDC)*** 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.

The Cambridge Structural Database

The world repository of small molecule crystal structures

==========

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.

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/

History of Crystallography and the Cambridge Structural Database

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.

Cambridge Structural Database
6 January 2014

CSD Entries: Summary Statistics

	Structures	%CSD
Total No. of structures	686 944	100.0
No. of different compounds	628 684	-
No. of literature sources	1 578	-
Organic structures	292 661	42.6
Transition metal present	369 682	53.8
Li – Fr or Be – Ra present	34 433	5.0
Main group metal present	41 711	6.1
3D coordinates present	643 032	93.3
Error-free coordinates	630 329	98.0†
Neutron studies	1 616	0.2
Powder diffraction studies	2 930	0.4
Low/high temp. studies	306809	44.7
Absolute configuration determined	14 752	2.1
Disorder present in structure	158 127	23.0
Polymorphic structures	20 753	3.0
R-factor < 0.100	645 809	94.0
R-factor < 0.075	585 333	85.2
R-factor < 0.050	378 391	55.1
R-factor < 0.030	78 594	11.4
No. of atoms with 3D coordinates	53 563 990	-

† Taken as a percentage of structures for which 3D coordinates are present in the CSD

https://www.ccdc.cam.ac.uk/

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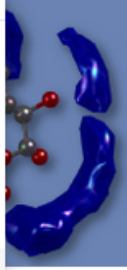
Community | Research & Consultancy | Solutions | News & Events | Support & Resources | The CCDC

Support & Resources

CSDS Downloads
Hosted Services
Documentation and Resources
CSD Python API Forum
Support
Downloads

The Cambridge Structural Database (CSD

The world's comprehensive and up-to-date database of crystal structures with over 875,000 fully curated entries



Available Now!

CSD 2017 – The world's repository for small-molecule crystal structures

Learn more about the different CSD software suites: **CSD-System**, **CSD-Discovery**, **CSD-Materials** and **CSD-Enterprise**

What's new for 2017? **2017 CSD updates** **Download CSD 2017**

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

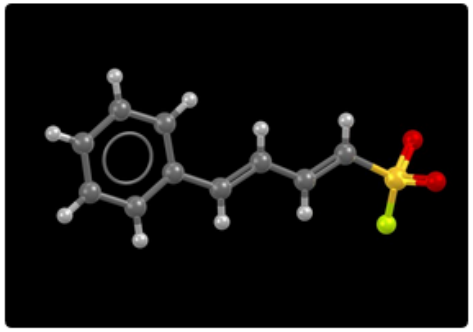
View and retrieve structures in the Cambridge Structural Database

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 enriched and included in the Cambridge Structural Database (CSD) which underpins a range of software solutions offered by CCDC. Targeted subsets of the CSD are also freely available to support teaching and other activities.

Tweets by @ccdc_cambridge

CCDC Cambridge @ccdc_cambridge

Today's #FeaturedStructureFriday is a novel structure from Prof. K. B. Sharpless; CSD refcode TATZAS dx.doi.org/10.5517/ccdc.c…



28 Apr

CCDC Cambridge @ccdc_cambridge

Embed View on Twitter

Access Structures

Entry search

Welcome to Access Structures the CCDC's free service to view and retrieve structures in the Cambridge Structural Database (CSD).

Please use one or more of the boxes to find entries in the CSD. If you enter details in more than one field the search will try to find records containing *all* the terms entered.
More information and search help

CCDC identifier(s) CCDC Number(s) or CSD refcodes(s)

Compound name e.g. sulfadiazine

DOI A single publication DOI or CSD DOI

Authors e.g. F.H.Allen

Journal e.g. Journal of the American Chemical Society

Publication details Year — Volume — Page

Search | I have none of the above | Clear

Advanced Search

Find structures in the Cambridge Structural Database using our advanced search functionality

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

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[b] *College of Liberal Arts and Sciences, Maryville University, St. Louis, MO 63141, USA*

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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.

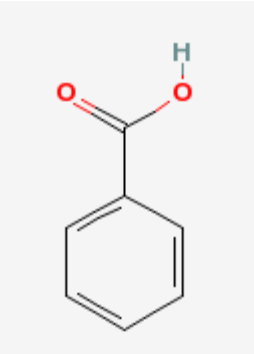
2. Supplementary data

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).

Benzoic acid:

βενζοϊκό οξύ, C_6H_5COOH.

Το απλούστερο αρωματικό οξύ

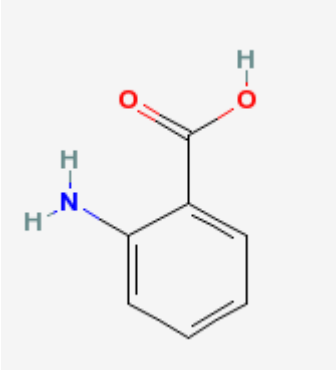


Aminobenzoic acid

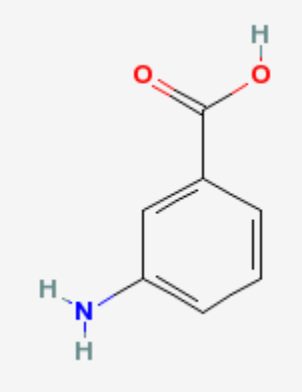
(benzoic acid with amine)

2-Aminobenzoic Acid

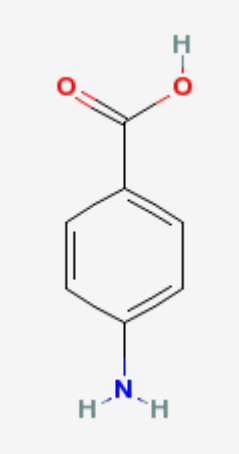
Anthranilic acid



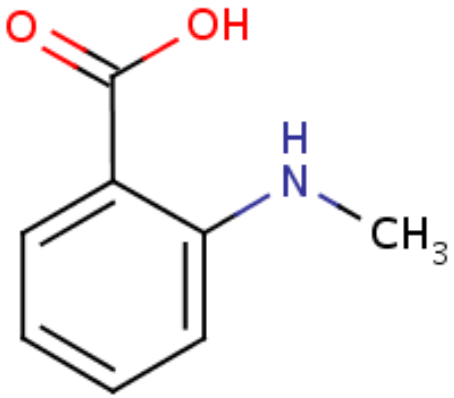
3-Aminobenzoic Acid



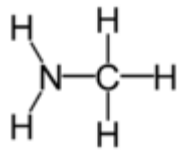
4-Aminobenzoic Acid



***N*-methylanthranilic acid**



methylamine



The host–guest complex

N-methylanthranilic acid (NAA) and β-cyclodextrin

in order to study the affects of N-substitution of aromatic aminobenzoic acids on crystal packing in the solid state.

CSD Entry: CUPYOC

Your query was: CCDC identifier(s): 735463 and the search returned 1 record.

New Search

Results

Refcode	CCDC Number
CUPYOC	735463

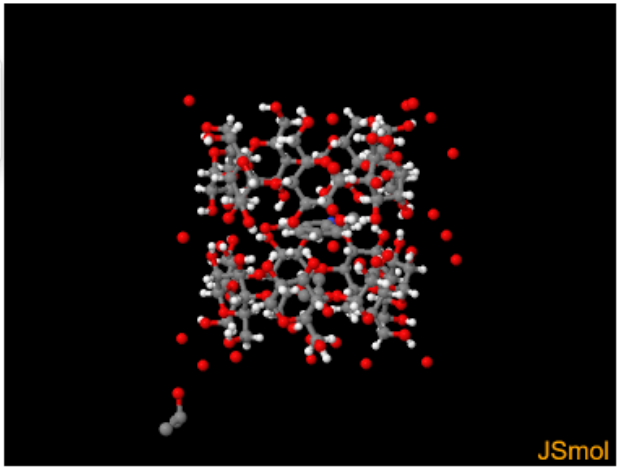
Download

Download current entry

Download all selected entries

CUPYOC : bis(β-Cyclodextrin) N-methylanthranilic acid isopropanol clathrate isopropanol solvate hydrate
Space Group: P1, **Cell:** *a* 15.2773(15)Å *b* 15.4710(15)Å *c* 17.9627(18)Å, *α* 99.632(5)° *β* 113.416(5)° *γ* 102.818(5)°

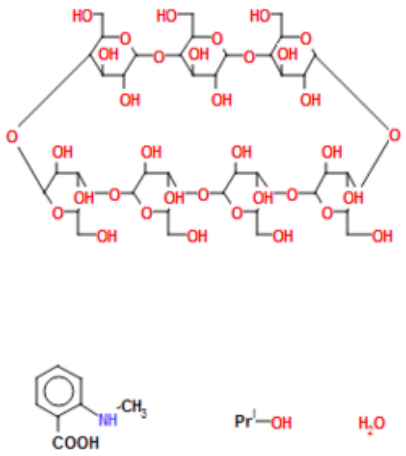
3D viewer



H | Disorder | Menu | Open

Style	Labels	Packing	Measure
Ball and Stick	No Labels	None	None

Chemical diagram



View group symbols key

Additional CCDC details

CCDC Number	735463
CCDC Citation	N.R.Lien, J.R.Telford CCDC 735463: Experimental Crystal Structure Determination, 2014, DOI: 10.5517/ccsp9mc
Deposited on	08/06/2009

Your query was: CCDC identifier(s): 7

New Search

Results

Refcode	CCDC Number
CUPYOC	735463

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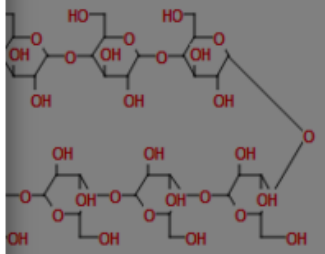
solvate hydrate
113.416(5)° γ 102.818(5)°



Style: Ball and Stick | Labels: No Labels | Packing: None | Measure: None

View group symbols key

Additional CCDC details

CCDC Number	735463
CCDC Citation	N.R.Lien, J.R.Telford CCDC 735463: Experimental Crystal Structure Determination, 2014, DOI: 10.5517/ccsp9mc
Deposited on	08/06/2009

Download deposited CIF

- (•) Deposited CIF(s)
- ( ) Deposited CIF(s) without structure factor data
- ( ) Deposited file(s) with any available structure factor data and checkCIF reports included

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*Το αρχείο κρυσταλλικής δομής **cif***

*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.

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
```

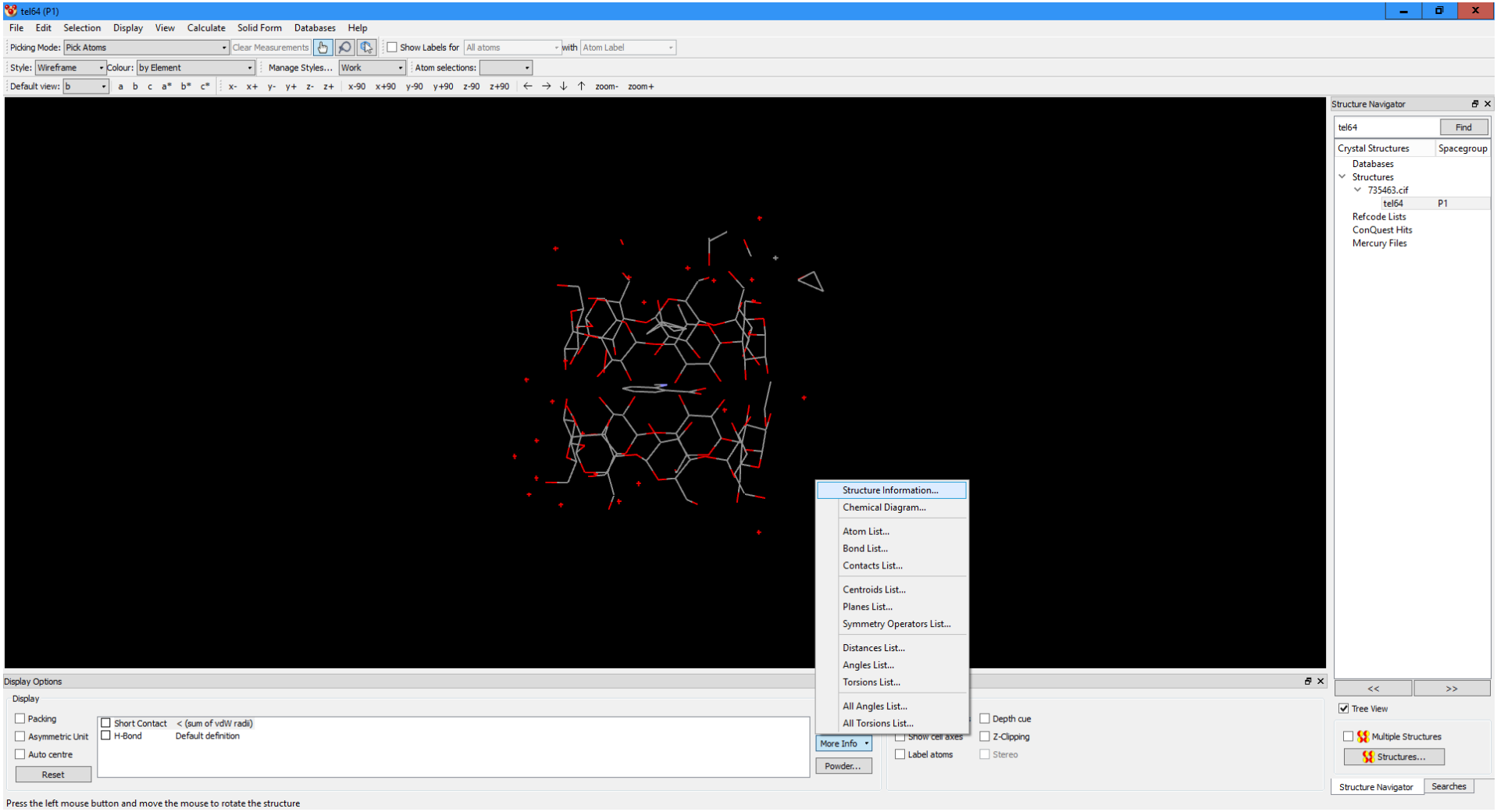
...

CIF

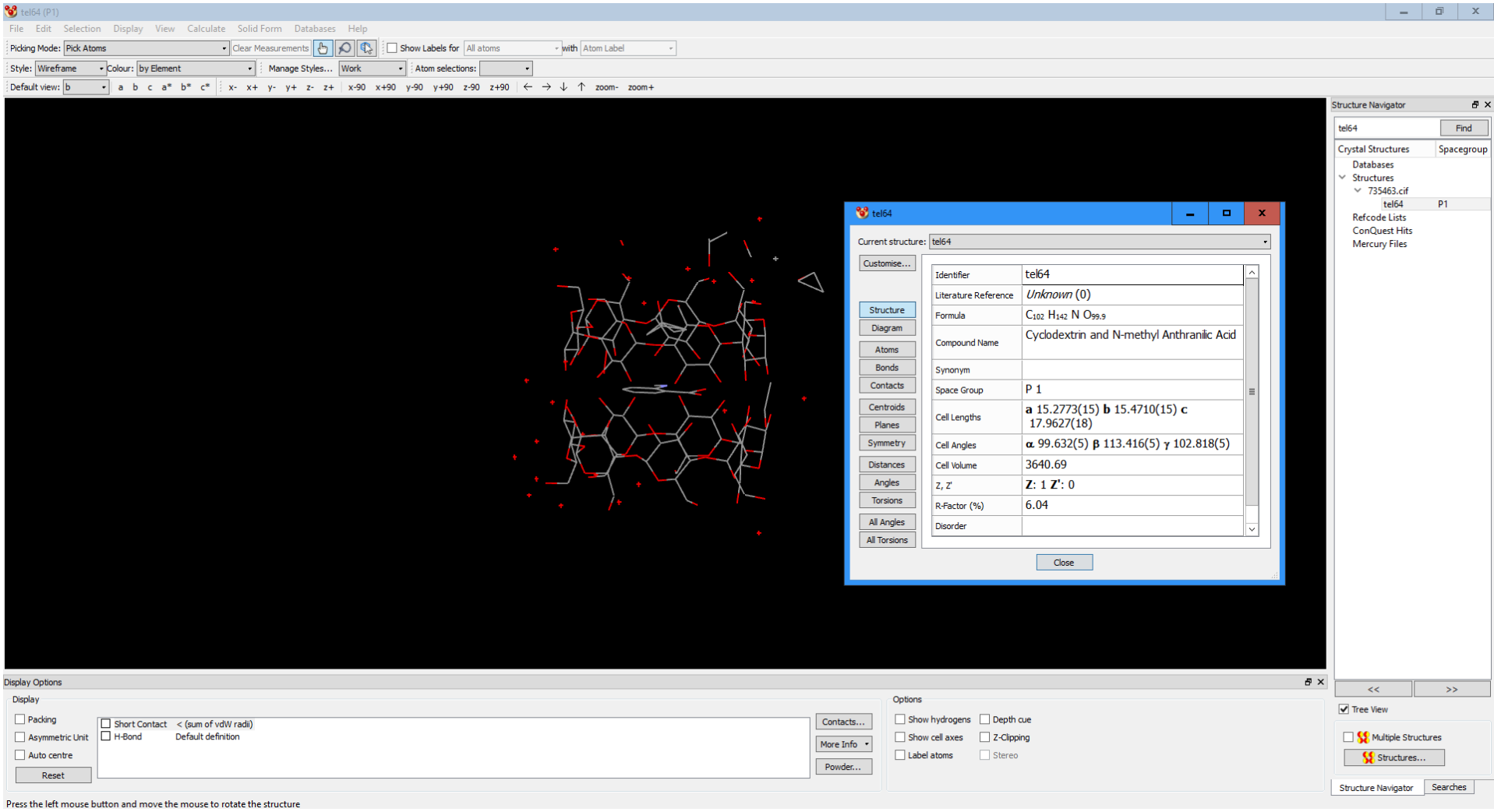
Structural info

```
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
…
```

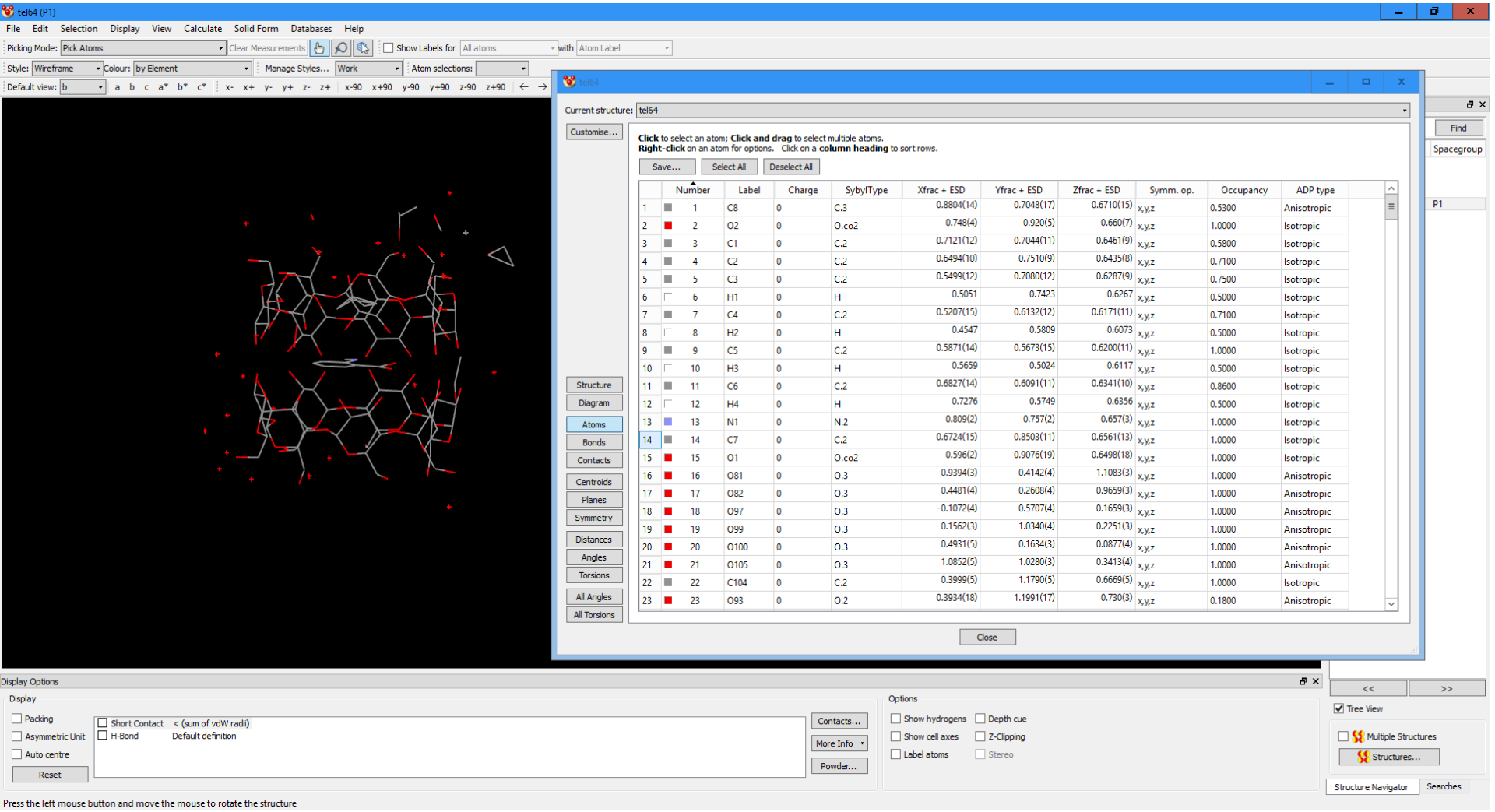
Program *Mercury*



Program ***Mercury***



Program *Mercury*



Παράδειγμα για εξοικείωση με το πρόγραμμα *Mercury*
https://www.ccdc.cam.ac.uk/support-and-resources/downloads/

1. Από Menu, Databases → Open the Teaching Subset →
→ Περιοχή Structure Navigator (δεξιά) → YILLAG

ή άνοιξε το file YILLAG.cif από το test_case folder

2. Display options (Options) → More Info → Structure Information
Γαλακτικό οξύ (Lactic acid) $CH_3CH(OH)COOH$

3. α) Περιοχή: Display options (Options) → Show hydrogens
β) Περιοχή: Display options (Options) → Show cell axes
γ) Περιοχή: Display options (Display) → Packing

δ) Γραμμή: Alignment and Orientation Operations "a b c a^* b* c* ..."
View along: a axis, b axis, ...

ε) Περιοχή: Display options (Display) → Reset

4.Toolbars κάτω από το Menu

α) Style

β) Colour

γ) Manage Styles

δ) Picking Mode

d [C1-C2] = ...

d [C2-O3] = ...

d [C1-O2] = ...

Angle [ ] = ...

Angle [ ] = ...

Angle [ ] = ...

Torsion Angle [O1 C1 C2 C3] = ...

Torsion Angle [ ] = ...

5. Contacts

α) Περιοχή: Display options (Display) → H-Bond

(Στην toolbar: Picking Mode έγινε Expand Contacts)

Γαλάζιες διακεκομμένες = expanded

Κόκκινες διακεκομμένες = not-expanded

Περιοχή: Display options (Display) → Reset

β) Περιοχή: Display options (Display) → Short Contact

Define short contacts

Contacts… button

Right click on short contacts

(Menu) Calculate → Contacts

6. (Menu) Calculate

α) Calculate → Centroids

(πρώτα, στην toolbar: Picking Mode βάλε Select Atoms)

Σχεδιάστε το centroid των ατόμων C1 C2 O1 O2 O3

β) Calculate → planes

(αφού πρώτα στην περιοχή Options επιλέξεις το Show cell axes, δοκίμασε τα hkl (1 0 0) (0 1 0) (1 1 1).

Βρες τη γωνία μεταξύ (1 0 0) και (0 1 0)

Βρες τη γωνία μεταξύ (1 0 0) και (1 1 1)

Βρες την απόσταση του centroid C1 C2 O1 O2 και plane (1 0 0)

7. (Menu) Display → Show/Hide → Centroids… Planes...

πρώτα, στην toolbar: Picking Mode βάλε Select Atoms

Σχεδίασε το mean plane που ορίζεται από τα άτομα: C1 C2 O1 O2 O3

Βρες τη γωνία μεταξύ (1 0 0) και mean plane [C1 C2 O1 O2 O3]

ΠΑΡΑΡΤΗΜΑ

The temperature factor

In a crystal structure an atom is bound to others by bond forces of various types. Their arrangement corresponds to an energy minimum. If the atoms are disturbed they will tend to return to the positions of minimal energy: they will oscillate around such positions gaining thermal energy.

The oscillations will modify the electron density function of each atom and consequently their capacity to scatter. Here we will suppose that the thermal motion of an atom is independent of that of the others. This is not completely true since the chemical bonds introduce strong correlations between the thermal motions of various atoms (see pp. 117–20 and Appendix 3.B, p. 186).

The time-scale of a scattering experiment is much longer than periods of thermal vibration of atoms. Therefore the description of thermal motion of an atom requires only the knowledge of the time-averged distribution of its position with respect to that of equilibrium. If we suppose that the position of equilibrium is at the origin, that $p(\boldsymbol{r}')$ is the probability of finding the centre of one atom at $\boldsymbol{r}'$, and that $\rho_a(\boldsymbol{r}-\boldsymbol{r}')$ is the electron density at $\boldsymbol{r}$ when the centre of the atom is at $\boldsymbol{r}'$, then we can write

$$\rho_{at}(\boldsymbol{r}) = \int_{S'} \rho_a(\boldsymbol{r}-\boldsymbol{r}')p(\boldsymbol{r}')\,\mathrm{d}\boldsymbol{r}' = \rho_a(\boldsymbol{r}') * p(\boldsymbol{r}') \qquad (3.15)$$

where $\rho_{at}(\boldsymbol{r})$ is the electron density corresponding to the thermically agitated atom. Notice that the rigid body vibration assumption has been made; i.e., the electron density is assumed to accompany the nucleus during thermal vibration.

In accordance with Appendix 3.A, p. 181), ρ_{at} is the convolution of two

functions and its Fourier transform (see eqn (3.A.38)) is

$$f_{at}(\boldsymbol{r}^*) = f_a(\boldsymbol{r}^*)q(\boldsymbol{r}^*) \tag{3.16}$$

where

$$q(\boldsymbol{r}^*) = \int_{S'} p(\boldsymbol{r}') \exp(2\pi i \boldsymbol{r}^* \cdot \boldsymbol{r}')\, d\boldsymbol{r}' \tag{3.17}$$

the Fourier transform of $p(\boldsymbol{r}')$, is known as the Debye–Waller factor.

The function $p(\boldsymbol{r}')$ depends on few parameters; it is inversely dependent on atomic mass and on chemical bond forces, and directly dependent on temperature. $p(\boldsymbol{r}')$ is in general anisotropic. If assumed isotropic, the thermal motion of the atom will have spherical symmetry and could be described by a Gaussian function in any system of reference:

$$p(\boldsymbol{r}') = p(r') \simeq (2\pi)^{-1/2} U^{-1/2} \exp[-(r'^2/2U)] \tag{3.18}$$

where r' is measured in Å and $U = \langle r'^2 \rangle$ is the square mean shift of the atom with respect to the position of equilibrium. The corresponding Fourier transform is (see eqn (3.A.25))

$$\begin{aligned} q(r^*) &= \exp(-2\pi^2 U r^{*2}) = \exp(-8\pi^2 U \sin^2\theta/\lambda^2) \\ &= \exp(-B \sin^2\theta/\lambda^2) \end{aligned} \tag{3.19}$$

where

$$B = 8\pi^2 U\ (\text{Å}^2).$$

The factor B is usually known in the literature as the **atomic temperature factor**.

The dependence of B on the absolute temperature T has been studied by Debye who obtained a formula valid for materials composed of only one chemical element. From X-ray diffraction structure analysis it is possible to conclude schematically that the order of value of $\sqrt{U}$ is in many inorganic crystals between 0.05 and 0.20 Å (B lying between 0.20 and 3.16 Å^2) but can also reach 0.5 Å ($B \simeq 20$ Å^2) for some organic crystals. The consequence of this is to make the electron density of the atom more diffuse and therefore to reduce the capacity for scattering with increasing values of $\sin\theta/\lambda$.

In general an atom will not be free to vibrate equally in all directions. If we assume that the probability $p(\boldsymbol{r}')$ has a three-dimensional Gaussian distribution the surfaces of equal probability will be ellipsoids called vibrational or thermal, centred on the mean position occupied by the atom.

Now eqn (3.19) will be substituted (see Appendix 3.B, pp. 186 and 188) by the anisotropic temperature factor (3.20) which represents a vibrational ellipsoid in reciprocal space defined by six parameters U_{11}^*, U_{22}^*, U_{33}^*, U_{12}^*, U_{13}^*, U_{23}^*:

$$q(\boldsymbol{r}^*) = \exp\left[-2\pi^2(U_{11}^* x^{*2} + U_{22}^* y^{*2} + U_{33}^* z^{*2} + 2U_{12}^* x^* y^* + 2U_{13}^* x^* z^* + 2U_{23}^* y^* z^*)\right]. \tag{3.20}$$

The six parameters U_{ij}^* (five more than the unique parameter U necessary to characterize the isotropic thermal motion) define the orientation of the thermal ellipsoid with respect to the crystallographic axes and the lengths of the three ellipsoid axes. In order to describe graphically a crystal molecule

Name:
'_atom_site_U_iso_or_equiv'

Definition:
Isotropic atomic displacement parameter, or equivalent isotropic atomic displacement parameter, U(equiv), in angstroms squared, calculated from anisotropic atomic displacement parameters.

U(equiv) = (1/3) sum~i~[sum~j~(U^ij^ a*~i~ a*~j~ a~i~ a~j~)]

a = the real-space cell lengths
a* = the reciprocal-space cell lengths

Ref: Fischer, R. X. & Tillmanns, E. (1988). Acta Cryst. C44, 775-776.

CIF

The acronym CIF is used both for the *Crystallographic Information File*, the data exchange standard file format of Hall, Allen & Brown (1991), and for the *Crystallographic Information Framework*, a broader system of exchange protocols based on data dictionaries and relational rules expressible in different machine-readable manifestations, including, but not restricted to, Crystallographic Information File and XML.

CIF was developed by the IUCr Working Party on Crystallographic Information in an effort sponsored by the IUCr Commission on Crystallographic Data and the IUCr Commission on Journals, and was adopted in 1990 as a standard file structure for the archiving and distribution of crystallographic information. It is now well established and is in regular use for reporting crystal structure determinations to *Acta Crystallographica* and other journals. It is often cited as a model example of integrating data and textual information for data-centric scientific communication.

Importance of CIF and the value of its accompanying web-based service for the validation of structural data, checkCIF

CIF and checkCIF are easily accessible and have served to make critical crystallographic data more consistently reliable and accessible at all stages of the information chain, from authors, reviewers and editors through to readers and researchers. In doing so, the system takes away the donkeywork from ensuring that the results of scientific research are trustworthy without detracting from the value of human judgement in the research and publication process.