

**Licence of Access Agreement to the Cambridge Structural Database
Academic Organisation**

An Agreement made between the Cambridge Crystallographic Data Centre (CCDC), [redacted] and [redacted]

University of California, San Diego
[redacted]



Dated: August 24, 2001

1. Subject to the restrictions detailed below, the CCDC will provide the Organisation with the material and facilities detailed in Part I of the Schedule to this Agreement.
2. At all times under this Agreement the copyright in and all other property rights and interests in the Cambridge Structural Database (CSD) and the associated CSD Software which jointly comprise the CSD System shall be and will remain with the CCDC. Modifications may be made by the Organisation to the CSD or to the CSD System on condition that:
 - a. Copyright in the modifications will vest in the CCDC which shall be entitled to obtain on its own behalf any available patent or similar protection and the Organisation shall execute any documents and do any acts necessary to vest such rights etc. in the CCDC;
 - b. The CCDC must be notified in writing, with full particulars (including explanations, manuals codes, etc.), of any and all modifications within three months of such modifications being effected.

The Organisation will take every reasonable precaution not to do or omit to do anything which prejudices the proprietary rights of the CCDC in the CSD or the CSD System.

3. The Licence to use the CSD and/or the CSD System applies to the calendar year 1 January 2001 to 31 December 2001 and will be renewed automatically unless either the CCDC or the Organisation cancels the agreement by 31st October of any calendar year. Financial arrangements, if any, are detailed in Part II of the Schedule to this Agreement. Any changes to the financial arrangements must be announced by the CCDC no later than the 30th September of each calendar year.
4. The Organisation is licensed to use the CSD and/or the CSD System subject to the following conditions:
 - 4.1. This Licence is personal to the Organisation who may not assign or sublease the same.
 - 4.2. Access to the CSD and CSD System shall be limited to the staff of the Organisation and visiting academic workers only at the location specified in Part III, and use of the CSD and the CSD System shall be limited to the computer specified in Part III of the Schedule to this Agreement.
 - 4.3. The CSD and the CSD System shall not be used in conjunction with any consulting or joint project with any non academic Organisation without prior written permission of the CCDC. Academic Organisations are defined as not-for-profit, or charitable Organisations, supported by private, charitable or Government funding, whose staff may freely publish the results of scientific research through the normal academic channels.
 - 4.4. The CSD and CSD System (including downloaded data, manuals, results and printed products) shall be used exclusively for the purpose of scientific teaching and research, which may include research such as, for example, into drug development or drug modifications capable of commercial exploitation. The results of such research may be published through the normal academic channels, subject to the inclusion of a proper acknowledgement to the CCDC (see Part IV of the Schedule to this Agreement).

4.5. The Organisation shall take every reasonable precaution to ensure that data held in the CSD or information derived or obtained from, or by the use of, the CSD or the CSD System is not (whether separately or in combination with other material) distributed or otherwise exploited (except through the product of scientific research as aforesaid) on a commercial or for-profit basis whether in printed, photographic, computer-readable or other form, without prior written permission from the CCDC. This restriction applies in particular, but not exclusively, to data compilations, educational aids, fragment libraries and software systems.

4.6. The Organisation may develop, for its own use, software systems based on the CSD or the CSD System or subfiles derived thereof. External distribution of such systems requires prior written permission of the CCDC.

5. The Organisation shall not copy (including indirectly) the CSD or CSD System or the documentation supplied in whole or in part or in any form whatsoever, whether machine readable or not, except for the purpose of generating backup copies.

6. The Organisation shall take every reasonable precaution to ensure that all persons permitted by the Organisation to have access to the CSD or CSD System shall comply with the conditions of this Agreement and shall take every reasonable precaution to ensure that paragraphs 2, 4 and 5 are adhered to. The provisions of paragraphs 2, 4, 5 and this paragraph 6 shall continue in force for 5 years after the termination of this Licence.

7. If computer-readable files are to be supplied, the information will be recorded by the CCDC on standard commercial recording media. In the event of the tapes or discs being received in damaged condition they will be replaced free of charge provided that the damaged tapes or discs are returned to the CCDC, accompanied by a covering letter explaining the nature of the damage.

8. The CCDC reserves the right to introduce major changes in the file and/or record structures and will give six months notice of such change.

9. Provided CCDC has complied with conditions set forth in FAR 52.233-1 - Disputes (Oct 1995), to the extent that the licensor is required by law to do so, CCDC shall have the right at any time to terminate this Agreement by notice in writing forthwith in the event that the Organisation should neglect or fail to observe any of its obligations under this Agreement. Notification shall be by certified mail, return receipt requested. A thirty day period following notification, prior to termination, will be provided to allow the Organisation to fulfil its obligations as defined in this agreement.

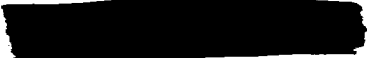
10. In the event that this Licence is terminated or is not renewed the Organisation shall return, or provide reasonable evidence of the destruction of, the CSD and/or CSD System supplied under this Agreement, and any backup copies and shall delete every part of the CSD and the CSD System from that Organisation's storage facilities.

11. Neither the CCDC nor any of its servants or agents shall be under any liability whatsoever (including without prejudice to generality of the foregoing any liability in contract or in tort or for consequential damage or loss of any kind) for any defect or error in, failure of, or unsuitability for any purpose of the CSD or CSD System or any part thereof or any extraneous material introduced therein and the Organisation accepts that there are no representations, warranties, conditions or liabilities expressed or implied herewith in relation to the supply of the CSD or the CSD System by the CCDC its servants or agents PROVIDED ALWAYS that nothing contained in this Licence shall or shall purport to exclude or limit liability where such exclusion or limitation is prohibited, void or unenforceable under the applicable Law as defined in Paragraph 13.

12. In the event that the CCDC is unable to continue to maintain the CSD System the copyright of the Database will be passed to the International Union of Crystallography.

13. This agreement shall be governed and interpreted in accordance with English Law as an English contract and English Courts shall have jurisdiction in respect of it. But, if use in the United States of the CSD System databases and software is arranged domestically under a federal contract, then US Federal Law, and the disputes procedure of that contract shall govern rather than the English Law and courts.

14. The Organisation warrants that it is an Academic Organisation as defined in this Agreement, and agrees to accept the Licence to use the CSD and/or CSD System on the terms set out in this Agreement.

Name:	Signature: 
Position:	Print Name: Karen Cargille
Date:	Position: AUL Technical Services
	Date: 24 August 2001

Schedule to the Licence of Access Agreement
Calendar Year 2002



Part I Items to be Supplied by the Cambridge Crystallographic Data Centre
The CSD 3D Graphics Search System, October 2001 and April 2002 releases

Part II Financial Arrangements
As invoiced by Wavefunction, Inc.

Part III Site/Computer Arrangements (to be completed in CAPITALS)

Full Address: [Redacted]

Primary Computer UNIX Linux PC Other

Operating System Windows 98 Pentium III

Secondary Computer UNIX Linux PC Other

Operating System WINDOWS 98 PENTIUM III

Part IV Acknowledgements

The following references should be quoted in all publications based on this Licence of Access:
3D Search and Research using the Cambridge Structural Database
Allen, F.H., Kennard, O., *Chemical Design Automation News* (1993), 8, 1 31-37.

IsoStar
Bruno, I.J., Cole, J.C., Lommerse, J.P.M., Rowland, R.S., Taylor, R. and Verdonk, M.L., *J. Computer-Aided Molec. Design*, 11, 525, 1997.

University of California, San Diego

Name: [Redacted] Signature: [Redacted]

Name: Dr David Hartley Print Name: Karen Cargille

Position: Executive Director Position: AUL Technical Services

Date: 20 DEC 2001 Date: 24 August 2001

Schedule to the Licence of Access Agreement
Calendar Year 2007



Part I Items Supplied (to be supplied by the Cambridge Crystallographic Data Centre)
The CSD 3D Graphics Search System, 2007 release (November 2006; including ConQuest, Mercury, PreQuest and Vista, IsoStar and Mogul).
Downloadable CSD data updates in 2007.

Part II Financial Arrangements

[Redacted]

Part III Site

[Redacted]

Organisation: University of California, San Diego

[Redacted]

Site: University of California, San Diego

[Redacted]

Computer Arrangements:

ConQuest/Mogul/Mercury installation on 1 only machine(s) (node-locked) and VISTA/IsoStar Client.

Version 5 System Software (including PreQuest, VISTA, IsoStar Server, Quest & SuperStar, where applicable)
(please tick boxes for installations on Primary/Secondary Computer and give the Operating System)

Primary Computer: Linux SGI Sun Operating System(s): WINDOWS

Secondary Computer: Linux SGI Sun Operating System(s): UNIX

Installation of the CSD System Version 5 Software on the Secondary Computer is permitted only in the event of the primary computer being inoperable for any reason, whereupon this licence shall be temporarily extended without additional charge to permit the installation of the CSD System on the Secondary Computer until such inoperability has been remedied provided that the Secondary Computer remains at all time under the direct control of the Organisation.

Part IV Acknowledgements

The following references should be quoted in all publications based on this Licence of Access:

The CSD System: The Cambridge Structural Database: A quarter of a million crystal structures and rising
F.H. Allen, *Acta Cryst.* (2002), **B58**, 380-388.
ConQuest: New software for searching the Cambridge Structural Database and visualizing crystal structures
I.J. Bruno, J.C. Cole, P.R. Edgington, M. Kessler, C.F. Macrae, P. McCabe, J. Pearson, R. Taylor, *Acta Cryst.* (2002), **B58**, 389-397.
Mercury: Mercury: visualization and analysis of crystal structures
C.F. Macrae, P.R. Edgington, P. McCabe, E. Pidcock, G.P. Shields, R. Taylor, M. Towler, J. van de Streek, *J. Appl. Cryst.* (2006), **39-3**, 453-457.
IsoStar: A library of information about nonbonded interactions
I.J. Bruno, J. Cole, J.P.M. Lommerse, R.S. Rowland, R. Taylor, M. Verdonk, *Journal of Computer Aided Molecular Design* (1997), **11-6**, 525-537.
Mogul: Retrieval of crystallographically derived molecular geometry information
I.J. Bruno, et al *Journal of Chemical Information and Computer Sciences* (2005), **44-6**, 2133-2144.
SuperStar: A knowledge-based approach for identifying interaction sites in proteins
M.L. Verdonk, J.C. Cole, R. Taylor, *Journal of Molecular Biology* (1999), **289**, 1093-1108.

For the CCDC

the Organisation

Signature:

[Redacted Signature]

Signature:

[Redacted Signature]

Name:

Dr Frank Allen

Name:

[Redacted Name]

Position:

Executive Director

Position:

HEAD, SERIALS RESOURCCE ACQ.

Date:

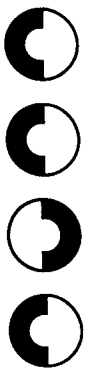
25 September 2006

Date:

10/23/06

The Cambridge Crystallographic Data Centre

Phone: [REDACTED]
 Fax: [REDACTED]
 E mail: [REDACTED]



Order Form for the Cambridge Structural Database System 2007

Organisation: University of California, San Diego

Site No.: [REDACTED] Confirmation Code: [REDACTED]

End User Contact Information

[REDACTED]
 University of California, San Diego
 [REDACTED]
 [REDACTED]
 [REDACTED]

Phone: [REDACTED]
 Fax: [REDACTED]
 E-mail: [REDACTED]

Please supply delivery address if different

Name: [REDACTED]
 Address: SAME
 [REDACTED]
 SAME

Please enter licence requirements for 2007

Access to the CSD System is provided exclusively under the terms of the Licence of Access Agreement, which permits access using a single computer only. The licence may be extended for access on additional computers, either individually or on a site wide, unlimited basis; additional fees payable are indicated below.	Qty	Unit Price (\$)	Total
Standard licence fee (single installation)	1	[REDACTED]	[REDACTED]
Additional licence(s)		[REDACTED]	
Unlimited site-wide access, additional fee	1	[REDACTED]	[REDACTED]
SuperStar		[REDACTED]	
1557401		Total	[REDACTED]

pd-co:
 10/23/06
 namat

Please return this order form and schedule to the CCDC with payment. Please select method of payment.

- payment by cheque, cheque enclosed
- payment by credit card on line at <http://www.ccdc.cam.ac.uk/usa>
 payment reference no. : _____
- by bank transfer to: [REDACTED]

Signature of Licensee's Authorised Representative

Print Name of Licensee's Authorised Representative

Date 10/23/06