

Licence of Access Agreement to the Cambridge Structural Database Academic Organisation

An Agreement made between the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge, United Kingdom, and

University of California, San Diego
Electronic Resources
Library
9500 Gilman Dr. 0175A
La Jolla, CA 02093



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).

*Cambridge
Structural
Database*

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.

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Name:

Position:

Date:

Executive Director
15/10/01

Signature

Print Name

Position:

Date:

AUL Technical Services

24 August 2001

Schedule to the Licence of Access Agreement Calendar Year 2008

Part I Items Supplied (to be supplied by the Cambridge Crystallographic Data Centre)
The CSD 3D Graphics Search System, 2008 Release (November 2007; including the CSD,
ConQuest, Mercury, PreQuest, Vista, IsoStar and Mogul) Downloadable CSD data updates in 2008
Materials module of Mercury

Part II Financial Arrangements
Organisation will pay CCDC **TEXT DELETED** (and any further payments due if upgraded access granted)

Part III Site

Organisation: University of California, San Diego
Electronic Resources
Library
9500 Gilman Drive 0175A
La Jolla, CA 92093
USA

Site: No: 1293 University of California, San Diego
La Jolla
CA 92093
USA

Computer Arrangements:

ConQuest/Mogul/Mercury installation on **unlimited** number of machine(s) (node-locked) and
VISTA/IsoStar Client.
(available on Windows, Linux, SGI, Sun & MacOSX- platform information not required on schedule)
Version 5 System Software (PreQuest/IsoStar Server/Quest/SuperStar where applicable) (please tick
boxes for installations on Primary/Secondary Computer and give the Operating System)

Version 5 Primary Computer: ☐Linux ☐SGI ☐Sun **Operating System:** _____
Version 5 Secondary Computer: ☐Linux ☐SGI ☐Sun **Operating System:** _____

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.

Site: No: 729 University of California, Berkeley
Berkeley
CA 94720
USA

Computer Arrangements:

ConQuest/Mogul/Mercury installation on **unlimited** number of machine(s) (node-locked) and
VISTA/IsoStar Client.
(available on Windows, Linux, SGI, Sun & MacOSX- platform information not required on schedule)
Version 5 System Software (PreQuest/IsoStar Server/Quest/SuperStar where applicable) (please tick
boxes for installations on Primary/Secondary Computer and give the Operating System)

Version 5 Primary Computer: ☐Linux ☐SGI ☐Sun **Operating System:** _____
Version 5 Secondary Computer: ☐Linux ☐SGI ☐Sun **Operating System:** _____

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.

Site: No: 731

University of California, Irvine
Irvine
CA 92717
USA

Computer Arrangements:

ConQuest/Mogul/Mercury installation on **unlimited** number of machine(s) (node-locked) and VISTA/IsoStar Client.
(available on Windows, Linux, SGI, Sun & MacOSX- platform information not required on schedule)
Version 5 System Software (PreQuest/IsoStar Server/Quest/SuperStar where applicable) (please tick boxes for installations on Primary/Secondary Computer and give the Operating System)

Version 5 Primary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

Version 5 Secondary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

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.

Site: No: 732

University of California, Riverside
Riverside
CA 92517
USA

Computer Arrangements:

ConQuest/Mogul/Mercury installation on **unlimited** number of machine(s) (node-locked) and VISTA/IsoStar Client.
(available on Windows, Linux, SGI, Sun & MacOSX- platform information not required on schedule)
Version 5 System Software (PreQuest/IsoStar Server/Quest/SuperStar where applicable) (please tick boxes for installations on Primary/Secondary Computer and give the Operating System)

Version 5 Primary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

Version 5 Secondary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

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.

Site: No: 1422

University of California, Los Angeles
Los Angeles
CA 90095
USA

Computer Arrangements:

ConQuest/Mogul/Mercury installation on **unlimited** number of machine(s) (node-locked) and VISTA/IsoStar Client.
(available on Windows, Linux, SGI, Sun & MacOSX- platform information not required on schedule)
Version 5 System Software (PreQuest/IsoStar Server/Quest/SuperStar where applicable) (please tick boxes for installations on Primary/Secondary Computer and give the Operating System)

Version 5 Primary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

Version 5 Secondary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

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.

Site: No: 1562

University of California, Santa Cruz
Santa Cruz
CA 95064
USA

Computer Arrangements:

ConQuest/Mogul/Mercury installation on **unlimited** number of machine(s) (node-locked) and VISTA/IsoStar Client.
(available on Windows, Linux, SGI, Sun & MacOSX- platform information not required on schedule)
Version 5 System Software (PreQuest/IsoStar Server/Quest/SuperStar where applicable) (please tick boxes for installations on Primary/Secondary Computer and give the Operating System)

Version 5 Primary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

Version 5 Secondary Computer: ☐Linux ☐SGI ☐Sun Operating System: _____

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 visualising 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, et al., *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, *J. Comput. Aid. Mol. Des.* (1997), **11**-6, 525-537.

Mogul: Retrieval of crystallographically derived molecular geometry information

I.J. Bruno, et al., *J. Chem. Inf. Comp. Sci.* (2004), **44**-6, 2133-2144.

SuperStar: A knowledge-based approach for identifying interaction sites in proteins

M.L. Verdonk, J.C. Cole, R. Taylor, *J. Mol. Biol.* (1999), **289**, 1093-1108.

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For the Organisation

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Signature

Signature:

Name:

Name:

Position:

Executive Director

Position:

Head of Acquisitions

Date:

3 Jan 2008

Date:

12/5/07