X D 2 0 0 6 - L I C E N C E A G R E E M E N T

This is an agreement between the **XD2006-GROUP**:

Anatoliy Volkov, Piero Macchi, Louis J. Farrugia, Carlo Gatti and Tibor Koritsanszky

and the **USER**, on the use and further development of

XD2006: A Computer Program Package for Multipole Refinement, Topological Analysis of Charge Densities and Evaluation of Intermolecular Energies from Experimental or Theoretical Structure Factors.

1. The receipt of a signed copy of this agreement from **USER** acknowledges that a copy of *XD2006* has been supplied to the USER.

2. The **XD2006-GROUP** will maintain and support *XD2006*, providing the **USER** with updates. Incremental releases and bug fixes of *XD2006* will be made available free of charge to **USER**, but some charge may be made for future major updates to the XD system.

3. The **XD2006-GROUP** hereby grants a licence to **USER** to use *XD2006* for purposes of research and to modify it under the following conditions:

a. **USER** will not supply a copy of the executables to anyone outside his/her institution for any reason whatsoever. This in no way limits his/her making of copies for backup purposes, or for running on more than one computer system at his/her institution. **USER**, however, may permit third parties to use *XD2006* on any system at his/her institution under his/her supervision. **USER** may disclose the documentation that relates to *XD2006*, for purposes of review, to third parties who contemplate the use of the software.

b. **USER** will not incorporate any part of *XD2006* into any other program system without written permission from the **XD2006-GROUP**.

c. Major modifications, improvements, developments and extensions (herein-after referred to as *changes*) must be discussed with the **XD2006-GROUP**. In such cases, the source code may be made available to the **USER**, who should inform the **XD2006-GROUP** on (i) all necessary details of the *changes* envisaged, (ii) the version of *XD2006* the *changes* are to be made and (iii) the time approximately needed to complete the work. The **XD2006-GROUP**, together with the subscribers will decide on the usefulness and feasibility of the *changes* proposed. The **XD2006-GROUP** retains its rights to make a final decision on the consent of such *changes*. If the **XD2006-GROUP** agrees to the *changes* made by **USER** it also guarantees to incorporate them into subsequent versions of *XD2006*.

4. **USER** understands that no large program such as *XD2006* can be "bug free", accordingly, *XD2006* is supplied on an "as is" basis, with no additional responsibility or liability. USER is requested to report on bugs to the **XD2006-GROUP** at :

xd-bugs@xd.chem.buffalo.edu

5. If results obtained by the use of *XD2006* are published, then **USER** agrees to acknowledge its use in an appropriate citation which reads:

" *XD2006 - a computer program for multipole refinement, topological analysis of charge densities and evaluation of intermolecular energies from experimental or theoretical structure factors*. Volkov, A.; Macchi, P.; Farrugia, L. J.; Gatti, C.; Mallinson, P.; Richter, T.; Koritsanszky, T.; (2006)."

Signed on behalf of **USER** :_____

Signed on behalf of **XD2006-GROUP** :_____

Your email address (for payment details)_____

Please return a signed copy of this agreement to :

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