



# LICENSE AGREEMENT - PURCHASE TERMS AND CONDITIONS

## (ACADEMIC LICENSE)

This Agreement includes Part 1 - CRYSTAL23 License agreement, Part 2 - License Purchase Terms and Conditions, and is the complete agreement for the Licensee to the purchase of a license, download and use of CRYSTAL23.

### Part 1: CRYSTAL23 License agreement

In the following,

- the term "the authors", is to be construed as meaning as the names as listed in the CRYSTAL23 User's Manual: *R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I.J. Bush, Ph. D'Arco, M. Llunell, M. Causà, Y. Noel, L. Maschio, A. Erba, M. Rérat, S. Casassa, B.G. Searle, J.K. Desmarais*
- the term "the managing authors" identifies the authors of CRYSTAL23 affiliated to the Theoretical Chemistry Group at the Department of Chemistry of the University of Torino, responsible for the maintenance, support, distribution, documentation, development and general management of the software: *S. Casassa, B. Civalleri, J. K. Desmarais, A. Erba, L. Maschio*
- the term "I" is referred to you as the end user licensee (Research Group leader) and "registered address" corresponds to the address of the end user licensee as specified during the registration process.

I request a copy of the ab initio code for periodic systems, CRYSTAL23. I will adhere to the following conditions upon receipt of the code.

1. I have the right to use CRYSTAL23 on more than one computer system at my registered address. If my registered address should change I will notify the new one to [info@crystalsolutions.eu](mailto:info@crystalsolutions.eu) and I will remove all copies of CRYSTAL23 from computer systems at the old address.
2. I will not supply a copy of the code to anyone for any reason whatsoever. This in no way limits my making copies of the code for backup purposes.
3. I am allowed to grant access to the executable modules to the researchers of my research group. I guarantee that all such users have read the original conditions for the supply of CRYSTAL23 and that they will comply with them.
4. I understand that copyright and intellectual property rights are retained by the authors.
5. I will not incorporate any part of CRYSTAL23 into any other program system, without prior written permission of the managing authors.
6. I will not attempt any software reverse engineering, such as decompilation, of CRYSTAL23.
7. I agree not to use CRYSTAL23 for profit-making purposes.

8. I understand that publications for which the CRYSTAL23 program is used must cite the following reference:

*A. Erba, J. K. Desmarais, S. Casassa, B. Civalleri, L. Donà, I. J. Bush, B. Searle, L. Maschio, L.-E. Daga, A. Cossard, C. Ribaldone, E. Ascrizzi, N. L. Marana, J.-P. Flament, B. Kirtman "CRYSTAL23: A Program for Computational Solid State Physics and Chemistry" J. Chem. Theory Comput. 2023, 19, 6891–6932  
<https://doi.org/10.1021/acs.jctc.2c00958>*

9. I understand that when using specific options of CRYSTAL23 I am invited to cite the relevant publications as found in the *CRYSTAL23 User's Manual* or/and in the CRYSTAL23 output file.

10. I understand that when referring to specific keywords and technical details of the CRYSTAL23 implementation I am invited to cite:

*R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I.J. Bush, Ph. D'Arco, M. Llunell, M. Causà, Y. Noel, L. Maschio, A. Erba, M. Rérat, S. Casassa, B.G. Searle, J.K. Desmarais "CRYSTAL23 User's Manual", University of Torino, Torino, 2023*

11. I understand that no large program such as CRYSTAL23 can be considered to be bug free, and accordingly the authors supply the software on an "as is" basis, with no additional responsibility or liability or warranty of merchantability or fitness for a particular purpose.

12. I agree to report any problems in the use of CRYSTAL23 to the managing authors ([crystal-support@unito.it](mailto:crystal-support@unito.it)).

## Part 2: Purchase Terms and Conditions

These are the terms and conditions according to which Aethia S.r.l. ("we" or "us") licenses end users ("you") the right to download and use CRYSTAL23.

### 1. CRYSTAL distribution

- i. CRYSTAL23 is distributed through the website <http://www.crystalsolutions.eu> within the agreement between the Department of Chemistry of the University of Torino and Aethia S.r.l.
- ii. CRYSTAL23 for Unix/Linux/MacOSX is supplied as binary executables or object files for a number of supported architectures (see <http://www.crystal.unito.it/platforms.php>).
- iii. CRYSTAL23 for Windows is supplied as a self-installing file and a Graphical User Interface.
- iv. Precompiled executables include sequential (crystal, properties, crystalOMP) and replicated data parallel versions (Pcrystal, Pproperties, PcrystalOMP). The massively-parallel versions (MPPcrystal, MPPcrystalOMP) are only supplied as object files.
- v. A web-based tool, CRYSPLOT, is freely available to visualize and plot properties computed with CRYSTAL (<http://crysplot.crystalsolutions.eu>). If you use it and make plots to be included in any publication please cite:

*G. Beata, G. Perego and B. Civalleri "CRYSPLOT: A New Tool to Visualize Physical and Chemical Properties of Molecules, Polymers, Surfaces, and Crystalline Solids" J. Comput. Chem. 40 (2019) 2329-2338*



## 2. Download

We will enable you to download CRYSTAL23 from the website <http://www.crystalsolutions.eu> after you have completed the "Check out" session and we have received the full payment. You will be able to download the purchased packages as many times as you like. In order to properly run CRYSTAL23, the computers where it will be downloaded and used shall run as their operating system either Windows (if you download the Windows version) or Unix/Linux/MacOSX (if you download the Unix/Linux/MacOSX version).

## 3. Restricted acts

You have no right to translate, adapt, arrange, decompile, modify, distribute and rent CRYSTAL23.

## 4. Payment

Aethia S.r.l. is not responsible for any bank fees associated with your method of payment. All prices are subject to change without notice.

## 5. Warranties

CRYSTAL23 is the outcome of academic work and its purpose is the study of periodic systems, as mentioned above, for scientific aims. Furthermore, no software program can be considered as bug free. Consequently, we license you CRYSTAL23 on an as-is basis without any warranty as to its functionality, to the fitness for any specific purpose and to the merchantability of its outputs; on the same ground, we will not be liable neither to you nor to any third party for any possible defect or malfunctioning. In any case, we invite you to report us for any problem in purchasing, downloading and using CRYSTAL23 to:

- [info@crystalsolutions.eu](mailto:info@crystalsolutions.eu): for supporting users with administrative questions (e.g. registration, quotation, payment, invoice, downloads, installation)
- [crystal-support@unito.it](mailto:crystal-support@unito.it): to help CRYSTAL23 users with problems related to execution, errors, input,...

## 6. Applicable law

This license and the connected rights are governed by, and shall be interpreted in accordance with, Italian law.

## 7. Disputes

Any dispute between you and us arising out of, or relating to, this license, the connected rights or CRYSTAL23 shall be deferred to one arbitrator who shall finally settle it in accordance with the arbitration rules of the "Camera Arbitrale del Piemonte". Seat of arbitration shall be Turin, Italy.

### 7.1 Online Dispute Resolution

The European Commission has set up an online platform that provides an alternative dispute resolution tool. <sup>[1]</sup><sub>[SEP]</sub>This tool can be used by the European consumer to solve out-of-court any dispute relating to and/or arising from online sales/purchases of goods and/or services. Therefore, if you are a European consumer, you can use this platform for the resolution of any dispute rising from the online contract with Aethia S.r.l. to purchase the CRYSTAL23 program. The platform is available at the following link: <http://ec.europa.eu/consumers/odr/>.

Aethia S.r.l. is available to answer any question submitted by email to the email address [info@crystalsolutions.eu](mailto:info@crystalsolutions.eu) <sup>[1]</sup><sub>[SEP]</sub>