

## LICENSE AGREEMENT - PURCHASE TERMS AND CONDITIONS (GOVERNMENT LICENSE)

This Agreement includes Part 1 - CRYSTAL17 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 CRYSTAL17.

### Part 1: CRYSTAL17 License agreement

*R. Dovesi, B. Civalleri, L. Maschio, A. Erba, S. Casassa  
Theoretical Chemistry Group – Department of Chemistry, University of Torino - Italy*

In the following, the term "the authors", is to be construed as meaning R. Dovesi, B. Civalleri, L. Maschio, A. Erba and S. Casassa at the above address, while 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, CRYSTAL17. I will adhere to the following conditions upon receipt of the code.

1. I have the right to use CRYSTAL17 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 CRYSTAL17 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. I will refer any requests for copies of the program to the authors.
3. I am allowed to grant access to the executable modules to the researchers of my research group at the government organization. I guarantee that all such users have read the original conditions for the supply of CRYSTAL17 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 CRYSTAL17 into any other program system, without prior written permission of the authors.
6. I will not attempt any software reverse engineering, such as decompilation, of CRYSTAL17.
7. Works in which the CRYSTAL17 program has been used should quote the following reference:

*R. Dovesi, A. Erba, R. Orlando, C. M. Zicovich-Wilson, B. Civalleri, L. Maschio, M. Rèrat, S. Casassa, J. Baima, S. Salustro, and B. Kirtman, "Quantum-Mechanical Condensed Matter Simulations with CRYSTAL17", WIREs Comput Mol Sci. e1360 (2018)  
<https://doi.org/10.1002/wcms.1360>*

(see the [www.crystal.unito.it](http://www.crystal.unito.it) web site for updated citations)

8. To refer to specific options and technical details of the CRYSTAL17 implementation please quote:

*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. Noël, L. Maschio, A. Erba, S. Casassa*  
"CRYSTAL17 User's Manual", University of Torino, Torino, 2017

9. References to specific algorithms as implemented in CRYSTAL17 can be found either at <http://www.crystal.unito.it> under the "Theoretical background" section or in the CRYSTAL17 output file.

It would be appreciated if a copy of such publications were sent to one of the authors (crystal@unito.it).

I understand that no large program such as CRYSTAL17 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. I agree to report any difficulties encountered in the use of CRYSTAL17 to the authors.

## 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 CRYSTAL.

### 1. CRYSTAL distribution

- i. CRYSTAL17 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. CRYSTAL17 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).
- iii. CRYSTAL17 for Windows is supplied as self extracting file, including the graphical package Crgra, and a Windows interface written to prepare the input and submit jobs.
- iv. Precompiled executables include sequential (crystal, properties) and replicated data parallel version (Pcrystal). The massive parallel version (MPPcrystal) is only supplied as object files.
- v. A new web-based tool, CRYSPLOT, is freely available to visualize and plot properties computed with CRYSTAL. If you use it and make plots to be included in any publication please quote:

*G. Beata, G. Perego and B. Civalleri "CRYSPLOT: a new tool visualize physical and chemical properties of periodic systems"*

*(see the <http://crysplot.crystalsolutions.eu> web site for updated citations)*

### 2. Download

We will enable you to download CRYSTAL17 from the website <http://www.crystalsolutions.eu> after you have completed the "Check out" session and we have received the full payment of the price for it. You will be able to download an indefinite number of executable copies. In order to properly run CRYSTAL07, 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 will not have any right neither to translate, adapt, arrange, decompile or anyhow modify CRYSTAL17, nor to distribute or rent CRYSTAL17.

### **4. Payment**

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

### **5. Warranties**

CRYSTAL17 is the outcome of academic work and the purpose of it 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 CRYSTAL17 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 CRYSTAL17 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 CRYSTAL17 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 CRYSTAL17 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. 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 Srl to purchase CRYSTAL17 program. The platform is available at the following link: <http://ec.europa.eu/consumers/odr/>.

Aethia Srl is available to answer any question submitted by email to the email address [info@crystalsolutions.eu](mailto:info@crystalsolutions.eu)