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### Part 1: CRYSTAL17 License agreement

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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 (Representative of the computer center), and "registered address" corresponds to the address of the computer center as specified during the registration process and "computer center" is considered to serve a single site.

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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. R  rat, 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](mailto: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.

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- 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)

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- [crystal-support@unito.it](mailto:crystal-support@unito.it): to help CRYSTAL17 users with problems related to execution, errors, input,...

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