Software License Agreement

between

—in the following referred to as "LICENSEE"—
and
Prof. Mihály Kállay, Budapest University of Technology and Economics
—in the following referred to as "LICENSOR"—

Preamble and Definitions

1. LICENSOR has developed a software-program "MRCC". "MRCC" is an experimental code for the accurate calculation of molecular energies and properties using ab initio and density functional quantum chemical methods.

2. LICENSEE can be an individual (personal license) or a non-commercial working organization, such as a university or another academic institution (site license).

3. The gratuitous non-exclusive granting (license) of "MRCC" will be effected under the following conditions.

§1 License

1. LICENSOR grants LICENSEE for the duration of this contract a non-exclusive license to use the software "MRCC" for non-commercial purposes.

2. Copyright for the source code and the documentation rests with the author, and source code and documentation are not being placed in the public domain.

   (a) The LICENSEE is required to make sure that only the "MRCC" executables, shell scripts, and utility programs are available to the users at the LICENSEE. The source and object files of the programs must be properly protected in order to prevent users from accessing them.

   (b) When the LICENSEE stops using a computer, proper actions will be taken to make sure that all "MRCC" - files, including object files and executables, are deleted on that computer.

   (c) All copies of "MRCC" will be deleted when it has ended its useful life.

   (d) Changes in the source code are only to be made in order to make the code compile and perform correctly on the site as well as to upgrade the code through patches supplied from the author. The source code may not be modified for other purpose without the written permission of the LICENSOR.

   (e) The "MRCC" source code may not, in whole or in part, be included in any program code LICENSEE distributes to other users, whether they have an "MRCC" license or not, without the specific written consent of the author of "MRCC".

   (f) The "MRCC" executable code may not be disassembled or reverse-engineered.

3. For the commercial use of the Software "MRCC" a separate agreement will be required.

4. LICENSEE does not have the right to assign the license to third parties or to grant sublicenses.

5. The documents and materials transferred from LICENSOR to the LICENSEE, including copies made thereof, remain the properties of LICENSOR.

§2 Confidentiality

1. LICENSEE promises to maintain in confidence the know-how provided to him by LICENSOR, in particular not to transfer it to third parties, and to use the know-how only in the scope of this agreement.

2. For this purpose LICENSEE will keep all documents and data carriers containing know-how of LICENSOR locked up in the same way as own secret documents, and LICENSEE will require all of its employees having access to the know-how and information of LICENSOR to sign a written confidentiality.

3. LICENSEE must not publish the Software as object code or as source code.

4. The above limitations do not apply to information

   (a) which LICENSEE already has in written form prior to signing this agreement,

(b) which have become accessible to the public due to publication of third parties without the activities of LICENSEE.

5. LICENSEE has the burden of proof for the existence of such exception.

§3 Payments

1. The license of Software "MRCC" or any part is for non-commercial use free of charge.
2. Transport and transmission costs will be covered by LICENSEE.

§4 Exclusion of liability

1. Users are to be informed that the experimental nature of this program means that there is no warranty of correctness of results nor fitness for a particular purpose and the author of "MRCC" cannot be held responsible in any way. The author of "MRCC" is not obliged to make corrections on reported errors, nor is there any support for users implied by making the program available.
2. The author will not provide a help line for usage problems.

§5 Copyright protection

1. The obligations by LICENSEE under this agreement are primarily in consideration for the transfer of secret know-how by LICENSOR and are not conditional upon the existence of copyright protection of the Software "MRCC".
2. The parties agree that the licensed Software "MRCC" has copyright protection.
3. LICENSOR does not guarantee the copyright protection of the licensed software or parts thereof.

§6 Copyright notice

1. The users must be informed that any published work arising from use of "MRCC" must include the following two citations:

   "D. Mester, P. R. Nagy, J. Csóka, L. Gyevi-Nagy, P. B. Szabó, R. A. Horváth, K. Petrov, B. Hégely, B. Ladóczki, G. Samu, B. D. Lőrincz, and M. Kállay: Overview of Developments in the MRCC Program System, *J. Phys. Chem. A* **129**, 2086 (2025)."

   "MRCC, a quantum chemical program suite written by M. Kállay, P. R. Nagy, D. Mester, L. Gyevi-Nagy, J. Csóka, P. B. Szabó, Z. Rolik, G. Samu, B. Hégely, B. Ladóczki, K. Petrov, J. Csontos, Á. Ganyecz, I. Ladjánszki, L. Szegedy, M. Farkas, P. D. Mezei, R. A. Horváth, and B. D. Lőrincz. See `www.mrcc.hu`."
2. Any published work arising from use of "MRCC" must also include citations to the scientific publications which describe the implementation and the underlying methodological developments. The corresponding references are given in Section 6 of document "Manual for the MRCC Program System", which is provided with the Software "MRCC".
3. If any input data for "MRCC" are generated by another program system, the users are also obliged to include an appropriate citation to the other program system as required by its authors.
4. If "MRCC" is used together with an external library, the users are also obliged to include an appropriate citation to the library as required by its authors.

§7 Developments of LICENSEE

1. LICENSEE will submit to LICENSOR any suggestions for improvements and further developments of "MRCC".
2. LICENSOR has the right to use the updates developed by LICENSEE, also beyond the termination of this agreement. This is also applicable in the case that LICENSEE obtains a patent for the improvement on "MRCC".
3. By the incorporation of improvements of LICENSEE into "MRCC" LICENSEE does not acquire any rights on this program and LICENSOR maintains the right to use these improvements within the Software "MRCC"

§8 Duration

This agreement is entered into for a duration of one year. It is extended automatically year by year unless it is terminated two months beforehand by one of the parties.

§9 Salvatorian clause

Should a provision of this agreement be invalid or become invalid or should this agreement contain an omission, then the legal effect of the other provisions shall not thereby be affected. Instead of the invalid provision a valid provision is deemed to have been upon which comes closest to what the parties intended commercially; the same applies in the case of an omission.

§10 Change to this agreement

Any change of this agreement requires written form, no collateral agreements to this agreement have been made.

§11 Jurisdiction and applicable law

The applicable law shall be that of the Republic of Hungary.

Budapest, Place and date

LICENSOR
Prof. Mihály Kállay

LICENSEE