IUPAC/InChI-Trust Licence for the International Chemical Identifier (InChI) Software ("IUPAC/InChI-Trust InChI Licence No. 1.0")

Copyright © IUPAC and InChI Trust Limited

This library is free software; you can redistribute it and/or modify it under the terms of the IUPAC/InChI Trust InChI Licence No. 1.0), or (at your option) any later version.

Terms and Conditions for Copying, Distribution and Modification of the InChI Software

0. This Licence Agreement applies to any software library or other program which contains a notice placed by the copyright holder or other authorized party saying it may be distributed under the terms of this Licence. The Licensee is addressed as "you".

'IUPAC' means the International Union of Pure and Applied Chemistry.

A "library" means a collection of software functions and/or data prepared so as to be conveniently linked with application programs (which use some of those functions and data) to form executables.

The "Library", below, refers to any such software library or work which has been distributed under these terms. A "work based on the Library" means either the Library or any derivative work under copyright law: that is to say, a work containing the Library or a portion of it, either verbatim or with modifications and/or translated straightforwardly into another language. (Hereinafter, translation is included without limitation in the term "modification".)

"Source code" for a work means the preferred form of the work for making modifications to it. For a library, complete source code means all the source code for all modules it contains, plus any associated interface definition files, plus the scripts used to control compilation and installation of the library.

Activities other than copying, distribution and modification are not covered by this Licence; they are outside its scope. The act of running a program using the Library is not restricted, and output from such a program is covered only if its contents constitute a work based on the Library (independent of the use of the Library in a tool for writing it). Whether that is true depends on what the Library does and what the program that uses the Library does.

1. You may copy and distribute verbatim copies of the Library's complete source code as you receive it, in any medium, provided that you conspicuously and appropriately publish on each copy an appropriate copyright notice and disclaimer of warranty; keep intact all the notices that refer to this Licence and to the absence of any warranty; and distribute a copy of this Licence along with the Library.

You may charge a fee for the physical act of transferring a copy, and you may at your option offer warranty protection in exchange for a fee.

- 2. You may modify your copy or copies of the Library or any portion of it, thus forming a work based on the Library, and copy and distribute such modifications or work under the terms of Section 1 above, provided that you also meet all of these conditions:
- a) The modified work must itself be a software library.
- b) You must cause the files modified to carry prominent notices stating that you changed the files and the date of any change.
- c) You must cause the whole of the work to be licensed at no charge to all third parties under the terms of this Licence. This requirement does not extend to any "work that uses the Library" that might also be compiled or linked against the "work based on the Library."
- d) If a facility in the modified Library refers to a function or a table of data to be supplied by an application program that uses the facility, other than as an argument passed when the facility is invoked, then you must make a good faith effort to ensure that, in the event an application does not supply such

function or table, the facility still operates, and performs whatever part of its purpose remains meaningful.

(For example, a function in a library to compute square roots has a purpose that is entirely well-defined independent of the application. Therefore, Subsection 2d requires that any application-supplied function or table used by this function must be optional: if the application does not supply it, the square root function must still compute square roots.)

These requirements apply to the modified work as a whole. If identifiable sections of that work are not derived from the Library, and can be reasonably considered independent and separate works in themselves, then this Licence, and its terms, do not apply to those sections when you distribute them as separate works. But when you distribute the same sections as part of a whole which is a work based on the Library, the distribution of the whole must be on the terms of this Licence, whose permissions for other Licensees extend to the entire whole, and thus to each and every part regardless of who wrote it.

Thus, it is not the intent of this section to claim rights or contest your rights to work written entirely by you; rather, the intent is to exercise the right to control the distribution of derivative or collective works based on the Library.

In addition, mere aggregation of another work not based on the Library with the Library (or with a work based on the Library) on a volume of a storage or distribution medium does not bring the other work under the scope of this Licence.

3. You may opt to apply the terms of the ordinary GNU General Public Licence instead of this Licence to a given copy of the Library. To do this, you must alter all the notices that refer to this Licence, so that they refer to the ordinary GNU General Public Licence, version 2, instead of to this Licence. (If a newer version than version 2 of the ordinary GNU General Public Licence has appeared, then you can specify that version instead if you wish.) Do not make any other change in these notices.

Once this change is made in a given copy, it is irreversible for that copy, so the ordinary GNU General Public Licence applies to all subsequent copies and derivative works made from that copy.

This option is useful when you wish to copy part of the code of the Library into a program that is not a library.

4. You may copy and distribute the Library (or a portion or derivative of it, under Section 2) in object code or executable form under the terms of Sections 1 and 2 above provided that you accompany it with the complete corresponding machine-readable source code, which must be distributed under the terms of Sections 1 and 2 above on a medium customarily used for software interchange.

If distribution of object code is made by offering access to copy from a designated place, then offering equivalent access to copy the source code from the same place satisfies the requirement to distribute the source code, even though third parties are not compelled to copy the source along with the object code.

- 5. A program that contains no derivative of any portion of the Library, but is designed to work with the Library by being compiled or linked with it, is called a "work that uses the Library". Such a work, in isolation, is not a derivative work of the Library, and therefore falls outside the scope of this Licence.
- 6. You may combine or link a "work that uses the Library" with the Library to produce a work containing portions of the Library, and distribute that work under terms of your choice.

You must give prominent notice with each copy of the work that the Library is used in it and that the Library and its use are covered by this Licence. You must supply a copy of this Licence. If the work during execution displays copyright notices, you must include the copyright notice for the Library among them, as well as a reference directing the user to the copy of this Licence. Also, you must do one of these things:

- a) Accompany the work with the complete corresponding machine-readable source code for the Library including whatever changes to the Library were used in the work (which must be distributed under Sections 1 and 2 above).
- b) Use a suitable shared library mechanism for linking with the Library. A suitable mechanism is one that (1) uses at run time a copy of the library already present on the user's computer system, rather than copying library functions into the executable, and (2) will operate properly with a modified version of the library, if the user installs one, as long as the modified version is interface-compatible with the version that the work was made with.
- c) Accompany the work with a written offer, valid for at least three years, to give the same user the materials specified in Subsection 6a, above, for a charge no more than the cost of performing this distribution.
- d) If distribution of the work is made by offering access to copy from a designated place, offer equivalent access to copy the above specified materials from the same place.
- e) Verify that the user has already received a copy of these materials or that you have already sent this user a copy.
- 7. You may place library facilities that are a work based on the Library side-by-side in a single library together with other library facilities not covered by this Licence, and distribute such a combined library, provided that the separate distribution of the work based on the Library and of the other library facilities is otherwise permitted, and provided that you do these two things:
- a) Accompany the combined library with a copy of the same work based on the Library, uncombined with any other library facilities. This must be distributed under the terms of the Sections above.
- b) Give prominent notice with the combined library of the fact that part of it is a work based on the Library, and explaining where to find the accompanying uncombined form of the same work.
- 8. You may not copy, modify, sublicense, link with, or distribute the Library except as expressly provided under this Licence. Any attempt otherwise to copy, modify, sublicense, link with, or distribute the Library is void, and will automatically terminate your rights under this Licence. However, parties who have received copies, or rights, from you under this Licence will not have their Licences terminated so long as such parties remain in full compliance.
- 9. You are not required to accept this Licence, since you have not signed it. However, nothing else grants you permission to modify or distribute the Library or its derivative works. These actions are prohibited by law if you do not accept this Licence. Therefore, by modifying or distributing the Library (or any work based on the Library), you indicate your acceptance of this Licence to do so, and all its terms and conditions for copying, distributing or modifying the Library or works based on it.
- 10. Each time you redistribute the Library (or any work based on the Library), the recipient automatically receives a Licence from the original licensor to copy, distribute, link with or modify the Library subject to these terms and conditions. You may not impose any further restrictions on the recipients' exercise of the rights granted herein. You are not responsible for enforcing compliance by third parties with this Licence.
- 11. If, as a consequence of a court judgment or allegation of patent infringement or for any other reason (not limited to patent issues), conditions are imposed on you (whether by court order, agreement or otherwise) that contradict the conditions of this Licence, they do not excuse you from the conditions of this Licence. If you cannot distribute so as to satisfy simultaneously your obligations under this Licence and any other pertinent obligations, then as a consequence you may not distribute the Library at all. For example, if a patent Licence would not permit royalty-free redistribution of the Library by all those who receive copies directly or indirectly through you, then the only way you could satisfy both it and this Licence would be to refrain entirely from distribution of the Library.

If any portion of this section is held invalid or unenforceable under any particular circumstance, the balance of the section is intended to apply, and the section as a whole is intended to apply in other circumstances.

It is not the purpose of this section to induce you to infringe any patents or other property right claims or to contest validity of any such claims; this section has the sole purpose of protecting the integrity of the free software distribution system which is implemented by public Licence practices. Many people have made generous contributions to the wide range of software distributed through that system in reliance on consistent application of that system; it is up to the author/donor to decide if he or she is willing to distribute software through any other system and a licensee cannot impose that choice.

This section is intended to make thoroughly clear what is believed to be a consequence of the rest of this Licence.

- 12. If the distribution and/or use of the Library is restricted in certain countries either by patents or by copyrighted interfaces, the original copyright holder who places the Library under this Licence may add an explicit geographical distribution limitation excluding those countries, so that distribution is permitted only in or among countries not thus excluded. In such case, this Licence incorporates the limitation as if written in the body of this Licence.
- 13. IUPAC and the InChI Trust Limited may publish revised and/or new versions of the IUPAC/InChI Trust Licence for the International Chemical Identifier (InChI) Software from time to time. Such new versions will be similar in spirit to the present version, but may differ in detail to address new problems or concerns.

Each version is given a distinguishing version number. If the Library specifies a version number of this Licence which applied to it and "any later version", you have the option of following the terms and conditions either of that version or of any later version published by IUPAC and the InChI Trust Limited.

- 14. If you wish to incorporate parts of the Library into other free programs whose distribution conditions are incompatible with these, write to the author to ask for permission.
- 15. If you modify the Library in any way whatsoever, the output from any such modified Library may not be referred to as 'InChI' or any similar name. Any attempt to refer to such output as 'InChI' will automatically terminate your rights under this Licence.

NO WARRANTY

- 16. Because the Library is licensed free of charge, there is no warranty for the Library, to the extent permitted by applicable law. Except when otherwise stated in writing the copyright holders and other parties provide the Library "as is" without warranty of any kind, either expressed or implied, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose. The entire risk as to the quality and performance of the Library is with you. Should the Library prove defective, you assume the cost of all necessary servicing, repair or correction.
- 17. In no event unless required by applicable law or agreed to in writing will any copyright holder, or any party who may modify and/or redistribute the Library as permitted above, be liable to you for damages, including any general, special, incidental or consequential damages arising out of the use or inability to use the Library (including but not limited to loss of data or data being rendered inaccurate or losses sustained by you or third parties or a failure of the Library to operate with any other software), even if such holder or other party has been advised of the possibility of such damages.

END OF TERMS AND CONDITIONS

Instructions for Use

You must attach the following notices to the library at the beginning of each source file - as a minimum each file needs to contain the "copyright" line and a link to the full notice.

[INSERT YOUR LIBRARY'S NAME AND ITS PURPOSE]

Copyright © [YEAR][COPYRIGHT OWNER]

This library is free software; you can redistribute it and/or modify it under the terms of the IUPAC/InChI Trust InChI Licence 1.0, or any later version.

Please note that this library is distributed WITHOUT ANY WARRANTIES whatsoever, whether expressed or implied. See the IUPAC/InChI Trust Licence for the International Chemical Identifier (InChI) Software ("IUPAC/InChI-Trust InChI Licence No. 1.0") for more details.

You should have received a copy of the IUPAC/InChI Trust InChI Licence No. 1.0 with this library; if not, please write to:

The InChI Trust 8 Cavendish Avenue Cambridge CB1 7US UK

or e-mail to alan@inchi-trust.org

In the event that you require anything else or have any questions, please write to:

[INSERT COPYRIGHT OWNERS DETAILS] [INSERT ADDRESS]

or contact us via email at: [INSERT EMAIL ADDRESS]

© 2011 IUPAC and InChI Trust Limited