

## **Agreement**

between

Technische Universität Kaiserslautern  
Gottlieb-Daimler-Straße  
67663 Kaiserslautern

for the Laboratory of Engineering Thermodynamics (LTD)  
Prof. Dr.-Ing. Hans Hasse

- hereinafter referred to as "LTD" -

and

the party identified in the order form

- hereinafter referred to as "User" -

regarding the Software "*ms2*" for molecular simulations. The term "Software" as referred hereinafter shall include all electronic and/or written information as described in the Annex. This definition explicitly includes all binary codes, libraries, source codes, compilation procedures and data files as well as electronic and/or printed documentation.

### **1 Eligibility**

The User must either be a natural person or an academic institution represented by a natural person.

### **2 Entering into a Contract**

2.1 In order to register as an "*ms2* User", it is necessary for the order form in the Internet presentation to be completed in full and then confirmed by clicking on the "proceed" button. The data will then be displayed again. If all the data are correct and complete, the registration data can be sent by clicking on the "order now" button. Clicking the "back / correct data" button brings you back to the page on which the registration data can be input and corrected. By sending the order form, a binding license offer is made.

- 2.2 After the order data have been recorded, the User will be given access to the download section of the *ms2* Internet presentation. The license agreement comes into existence when the User is notified by LTD about his access authorization.
- 2.3 The binding license offer that has been given will be sent to the User automatically via e-mail and can also be stored as a pdf document, which will be generated by clicking the "Generate pdf-file as order confirmation" button.
- 2.4 The contractual terms can be downloaded via the order form.
- 2.5 After leaving the order level, the order to LTD can no longer be retrieved online.
- 2.6 LTD shall store and use the information given in this manner to process the requested license agreement.
- 2.7 The Contract shall be subject to German law. The UN Convention on the International Sale of Goods shall be excluded.
- 2.8 Any general terms of business which the User may have shall not apply.
- 2.9 This Agreement may be terminated by both parties on giving six weeks' notice to the end of a week. Notice of termination must be in text form.

### **3 License**

- 3.1 LTD, as Licensee of the Software, hereby grants to the User the simple, nontransferable, non-further-sublicensable and nonexclusive sublicensing right to download and use the Software in the object code such as in the source code and also the accompanying material from the LTD server. The User shall be entitled to adapt modify and copy the Software in the context of this Contract. All provisions of the present Contract regarding the original Software will also apply to the Software as modified by the User. This granting of a right of use shall not involve any further acquisition of rights in respect of the Software.

Any use of the Software shall only be for purposes of research and academic teaching. Use in connection with a business purpose is not permitted. Transferring the Software to third parties is not allowed.

3.2 It shall be possible to use the results obtained with the Software in cooperations with third parties if the use takes place only for teaching or research purposes and no clauses of the present agreement are violated.

3.3 There is no license or registration fee.

#### **4 Revocation**

4.1 Users who are regarded as consumers for the purposes of Section 13 of the German Civil Code (Bürgerliches Gesetzbuch - BGB) shall have a right of revocation.

4.2 The right of revocation shall in principle apply for two weeks. The time limit for revocation shall commence on receipt of the access authorization notification. Revocation can be given in text form. In order to comply with the time limit, it is sufficient for the revocation to be sent at the proper time. The revocation does not need to contain any reasons.

4.3 In the event of revocation, the User shall delete all data supplied (in particular the download code) on the User's own data carriers, and in particular on all computers on which the User has stored the data. At LTD' request, this deletion shall be confirmed by affidavit.

#### **5 Guarantee and Liability**

5.1 LTD shall provide the Software without any guarantee obligation or any warranty as to its features and gives no guarantee that the Software is free from faults or that the Software is suitable for any particular purpose. In particular there will be no warranty that the Software will not infringe any Patent, Copyright, Trademark or other Intellectual Property Rights of third parties.

- 5.2 LTD shall be liable only in respect of gross negligent or deliberate acts. Any liability for consequential damage and pecuniary loss shall be excluded.

## **6 Obligations on the part of the User**

- 6.1 The User shall take appropriate precautions to protect the Software and his password from unauthorized access by third parties. The User shall notify any employees that it is not permitted to make copies in excess of the contractual amount.
- 6.2 The User shall make reference to the Software in all publications connected in any means with the Software. In journal publications proper reference to the paper has to be made in which the used version of the Software is described. That paper is specified in the download section of the download section of the internet presentation and in the source code. Any breach by the User of said obligations shall entitle LTD to terminate the Contract on an extraordinary basis.
- 6.3 The User shall immediately notify LTD of any faults of the Software.
- 6.4 Where the use of software belonging to a third party is necessary in order to operate the Software, the User shall ensure that the rights of use necessary for this purpose have been granted to the User before use.
- 6.5 The User is encouraged but not obliged to inform LTD about contributions and results, in particular adaptations of the Software and new programs, arising in connection with the Software.

## **7 Return**

When the Contract comes to an end, the User shall fully and finally delete copies of the Software provided by LTD. At LTD's request, this deletion shall be confirmed by affidavit.

## **8 Data Protection**

The data contained in the registration form shall be stored for the purpose of processing this Agreement. The User consents to this storage. This consent

may be revoked at any time. The stored data shall be sent to the User by email on request at any time. The data shall not be sold or passed on to third parties who are not part of LTD. LTD may pass on the User's name to other users.

## **9 Amendments to the Contract, Saving Clause**

- 9.1 This Contract contains all arrangements made between the parties in respect of the subject-matter of the Contract. No oral or written ancillary agreements exist. Amendments and additions to this Contract, including to this written form clause itself, must be in written form.
- 9.2 If one or more provisions of this Contract are invalid on the basis of mandatory legal provisions or for other reasons, the validity of the remaining contractual provisions shall not be affected thereby. The parties undertake to replace any such invalid provisions with new valid Agreements which approximate as closely as possible to the purpose of the Contract.

## Annex

### Description of the Software

1. Source code files
  - a. ms2.F90
  - b. ms2\_accumulator.F90
  - c. ms2\_component.F90
  - d. ms2\_ensemble.F90
  - e. ms2\_global.F90
  - f. ms2\_interaction.F90
  - g. ms2\_molecule.F90
  - h. ms2\_potential.F90
  - i. ms2\_simulation.F90
  - j. ms2\_site.F90
  - k. ms2\_stopwatch.F90
  - l. Makefile.mult
2. Auxiliary bash scripts for *ms2*
3. Java-Applets *ms2par* and *ms2chart*
4. Visualization software *ms2molecules*
5. Simulation examples
6. Electronic and/or printed documentation as available