CHEMSHELL PROGRAM SUITE

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[1] ChemShell, a Computational Chemistry Shell, see www.chemshell.org

If the program has been locally modified, the nature of the modifications should be outlined. If the QM/MM implementation within ChemShell has been used to obtain the results, please provide a citation to the following publication

[2] "QUASI: A general purpose implementation of the QM/MM approach and its application to problems in catalysis"

 P. Sherwood, A. H. de Vries, M. F. Guest, G. Schreckenbach, C. R. A. Catlow, S. A. French, A. A. Sokol, S. T. Bromley, W. Thiel, A. J. Turner, S. Billeter, F. Terstegen, S. Thiel, J. Kendrick, S. C. Rogers, J. Casci, M. Watson, F. King, E. Karlsen, M. Sjovoll, A. Fahmi,   A. Schafer, Ch. Lennartz, J. Mol. Struct. (Theochem.) 2003, 632, 1.

mentioning, where appropriate the authors of the specific programs used.

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6.1 This Agreement will take effect and the Licence Period will start when a completed copy of this Agreement, signed on behalf of the Licensee, and the amount of the then current licence fee has been received, in cleared funds, by STFC at the address given for this purpose on the Chemshell Website at the time the Licensee downloads this form of Licence Agreement from that website.

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7. **GENERAL**

7.1 **Headings:** The headings in this Agreement are for ease of reference only; they do not affect its construction or interpretation.

7.2 **Assignment etc:** The Licensee may not assign or transfer this Agreement as a whole, or any of its rights or obligations under it, without first obtaining the written consent of STFC.

7.3 **Illegal/unenforceable provisions:** If the whole or any part of any provision of this Agreement is void or unenforceable in any jurisdiction, the other provisions of this Agreement, and the rest of the void or unenforceable provision, will continue in force in that jurisdiction, and the validity and enforceability of that provision in any other jurisdiction will not be affected.

7.4 **Waiver of rights:** If STFC fails to enforce, or delays in enforcing, an obligation of the Licensee, or fails to exercise, or delays in exercising, a right under this Agreement, that failure or delay will not affect its right to enforce that obligation or constitute a waiver of that right. Any waiver by STFC of any provision of this Agreement will not, unless expressly stated to the contrary, constitute a waiver of that provision on a future occasion.

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SIGNED for and on behalf of the Licensee:

Name:

Position:

Signature:

Date:

THE APPENDIX

GNU General Public Licence

Version 2, June 1991

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