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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.

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Position:

Signature:

Date:

THE APPENDIX

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Version 2, June 1991

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