

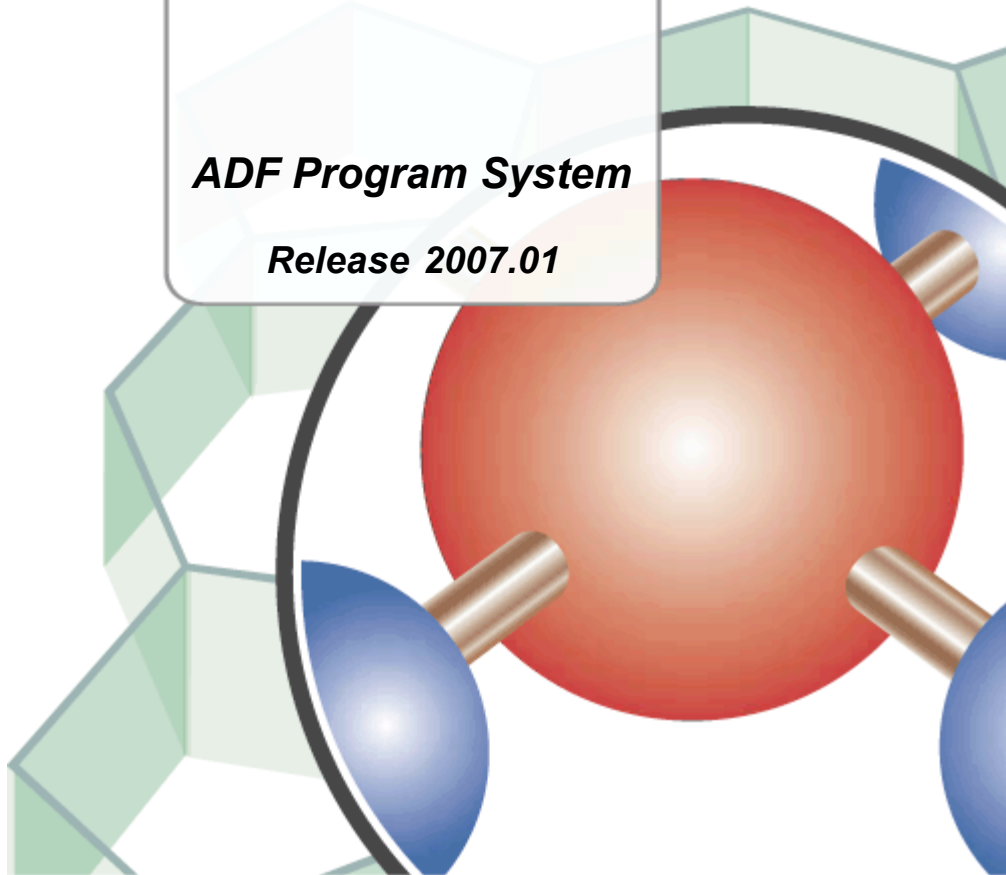


Scientific Computing & Modelling

# ***References***

***ADF Program System***

***Release 2007.01***



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## General References

When you publish results in the scientific literature that were obtained with programs of the ADF package, you are required to include references to the program package with the appropriate release number, and a few key publications.

In addition to these general references, references to special features are mandatory, in case you have used them. See the section [Feature References ADF](#) and [Feature References BAND](#).

## ADF

For calculations with the molecular ADF code, version 2007.01:

1. G. te Velde, F.M. Bickelhaupt, S.J.A. van Gisbergen, C. Fonseca Guerra, E.J. Baerends, J.G. Snijders, T. Ziegler, 'Chemistry with ADF', *J. Comput. Chem.* **22**, 931-967 (2001)
2. C. Fonseca Guerra, J.G. Snijders, G. te Velde, and E.J. Baerends, *Theor. Chem. Acc.* **99**, 391 (1998)
3. ADF2007.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

Optionally, you may add the following list of authors and contributors:

E.J. Baerends, J. Autschbach, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, S.J.A. van Gisbergen, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, G. van Kessel, F. Kootstra, E. van Lenthe, D.A. McCormack, A. Michalak, J. Neugebauer, V.P. Nicu, V.P. Osinga, S. Patchkovskii, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, P. Ros, P.R.T. Schipper, G. Schreckenbach, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo, A.L. Yakovlev, and T. Ziegler

Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

## BAND

For calculations with the periodic structures BAND code, version 2007.01:

1. G. te Velde and E.J. Baerends, *Phys. Rev B* **44**, 7888 (1991)
2. G. Wiesenekker and E.J. Baerends, *J. of Phys.: Condensed Matter* **3**, 6721 (1991)
3. BAND2007.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

Optionally, you may add the following list of authors and contributors:

G. te Velde, E.J. Baerends, P.H.T. Philipsen, G. Wiesenekker, J.A. Groeneveld, J.A. Berger, P.L. de Boeij, R. Klooster, F. Kootstra, P. Romaniello, J.G. Snijders, E.S. Kadantsev, T. Ziegler

Note: if you have used a modified (by yourself, for instance) version of the code, you should mention in the citation that a modified version has been used.

## **COSMO-RS**

For calculations with the COSMO-RS code, version 2007.01:

1. C. Pye, J. Louwen, E. van Lenthe, in preparation
2. ADF2007.01 COSMO-RS, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>

## Feature References ADF

When you have used special features, you should include one (or more, as the case may be) lead reference(s) to the implementation. Additional references to related publications are suggested.

### Geometry optimizations, transition states, and reaction paths

#### Transition State search

L. Versluis and T. Ziegler, *J. Chem. Phys.* **88**, 322 (1988)

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##### Lead references

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E. van Lenthe, R. van Leeuwen, E.J. Baerends, and J.G. Snijders, *Int. J. Quantum Chem.* **57**, 281 (1996)

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P.M. Boerrigter, E.J. Baerends, J.G. Snijders, *Chem. Phys.* **122**, 357 (1988)

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#### Lead

T. K. Woo, L. Cavallo, and T. Ziegler, *Theor. Chem. Acc.* **100**, 307 (1998)

#### Suggested

T. K. Woo, S. Patchkovskii, and T. Ziegler, *Computing in Science & Engineering*, 2000, November/December, 28-37

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M. Swart, *Int. J. Quant. Chem.*, 2003, **91**, 177

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### DRF

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### MM Dispersion

S. Grimme, *J. Comput. Chem.* **25**, 1463. (2004)

contact J.M. Ducere, L. Cavallo, University of Salerno, Italy, article in preparation.

## Molecular properties with ADF

### Frequencies, IR Intensities, Raman, VCD

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S.J.A van Gisbergen, J.G. Snijders, and E.J. Baerends, Comput. Phys. Commun. **118**, 119, (1999)

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Lead reference

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A. Rosa, E.J. Baerends, S.J.A. van Gisbergen, E. van Lenthe, J.A. Groeneveld, and J.G. Snijders, *J. Am. Chem. Soc.* **121**, 10356 (1999)

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## **Polarizabilities**

Lead

S.J.A van Gisbergen, J.G. Snijders, and E.J. Baerends, *J. Chem. Phys.* **103**, 9347 (1995)

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V.P. Osinga, S.J.A van Gisbergen, J.G. Snijders, and E.J. Baerends, *J. Chem. Phys.* **106**, 5091 (1997)

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Suggested:

S.J.A van Gisbergen, J.G. Snijders, and E.J. Baerends, *Phys. Rev. Lett.* **78**, 3097 (1997)

## **Dispersion Coefficients**

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V.P. Osinga, S.J.A van Gisbergen, J.G. Snijders, and E.J. Baerends, *J. Chem. Phys.* **106**, 5091 (1997)

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Lead

J. Autschbach, T. Ziegler, J. Chem. Phys. **116**, 891 (2002)

J. Autschbach, T. Ziegler, S.J.A van Gisbergen, and E.J. Baerends J. Chem. Phys. **116**, 6930 (2002)

## Optical Rotation (OR), Optical Rotation Dispersion (ORD)

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J. Autschbach, T. Ziegler, J. Chem. Phys. **116**, 891 (2002)

J. Autschbach, S. Patchkovskii, T. Ziegler, S.J.A. van Gisbergen, and E.J. Baerends, J. Chem. Phys. **117**, 581 (2002)

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Lead reference

G. Schreckenbach and T. Ziegler, J. Phys. Chem. **99**, 606 (1995)

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R.M. Dickson and T. Ziegler, J. Phys. Chem. **100**(13), 5286 (1996)

J. Khandogin and T. Ziegler, Spectrochimica Acta **55**, 607 (1999)

J. Autschbach, T. Ziegler, J. Am. Chem. Soc. **123**, 3341 (2001)

J. Autschbach, T. Ziegler, J. Am. Chem. Soc. **123**, 5320 (2001)

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J. Autschbach, T. Ziegler, in *Encyclopedia of Nuclear Magnetic Resonance*, Eds. D.M. Grant, R. K. Harris, John Wiley and Sons, Chichester, 2002, Vol. 9 *Advances in NMR*.

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### G-tensor: Zeeman interaction

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G. Schreckenbach and T. Ziegler, J. Phys. Chem. A 1997, **101**, 3388 (for ESR/EPR g-tensor)

S. Patchkovskii and T. Ziegler, J. Phys. Chem. A 2001, **105**, 5490 (for high-spin ESR/EPR g-tensor)

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Lead reference

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Lead reference (in ESR called Q-tensor: Nuclear electric quadrupole hyperfine interaction)

E. van Lenthe and E.J. Baerends, J. Chem. Phys **112**, 8279-8292 (2000)

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### Bond Energy Analysis

T. Ziegler and A. Rauk, Inorg. Chem. **18**, 1558 (1979)

T. Ziegler and A. Rauk, Inorg. Chem. **18**, 1755 (1979)

F M Bickelhaupt and E.J. Baerends, In: Rev. Comput. Chem.; K B Lipkowitz and D B Boyd, Eds.; Wiley, New York, 2000, Vol. 15, p.1-86

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E. S. Kadantsev, R. Klooster, P. L. de Boeij, and T. Ziegler, Mol. Phys. (accepted for publication) (2007).

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F. Kootstra, P.L. de Boeij, and J.G. Snijders, J. Chem. Phys. **112**, 6517 (2000).

P. Romaniello, and P.L. de Boeij, Phys. Rev. **B71**, 155108 (2005)

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F. Kootstra, Ph.D. thesis, Rijksuniversiteit Groningen, Groningen (2001).

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## Relativistic TDDFT

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## ADF-GUI and BAND-GUI

The ADF-GUI and BAND-GUI have been developed within SCM (with O. Visser as primary developer).

Main contributions outside SCM have come from:

P. Leyronnas, W.-J. van Zeist, and M. Luppi.

If you used the ADF-GUI (for example ADFview) you may optionally include the reference:

ADF-GUI 2007.01, SCM, Amsterdam, The Netherlands, [www.scm.com](http://www.scm.com)

Likewise if you used the BAND-GUI you may optionally include the reference:

BAND-GUI 2007.01, SCM, Amsterdam, The Netherlands, [www.scm.com](http://www.scm.com)