

LIST OF PUBLICATIONS

1. R. Burcl and P. Hobza, "Ab initio study on the methanol-water cation radical potential energy surface", *Theor. Chim. Acta* **87**, 97 - 105 (1993).
2. J. Šponer, R. Burcl and P. Hobza, "Interactions Between Amino Groups in DNA. An Ab Initio Study and a Comparison with Empirical Potentials", *J. Biomol. Struct. Dynamics* **11**, 1357 - 1376 (1994).
3. P. Hobza, R. Burcl, V. Špirko, O. Dopfer, K. Müller-Dethlefs and E. W. Schlag, "Ab initio study of the phenol-water cation radical", *J. Chem. Phys.* **101**, 990 - 997 (1994).
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5. R. Burcl, G. Chałasiński, R. Bukowski and M. M. Szczyński, "On the role of bond functions in interaction calculations. Ar...HCl, Ar...H₂O, (HF)₂", *J. Chem. Phys.* **103**, 1498 - 1507 (1995).
6. R. Burcl, S. M. Cybulski, M. M. Szczyński and G. Chałasiński, "Towards an analytical three-body potential of Ar₂Cl", *J. Chem. Phys.* **103**, 299 - 308 (1995).
7. S. M. Cybulski, R. Burcl, G. Chałasiński and M. M. Szczyński, "Partitioning of interaction energy in van der Waals complexes involving excited state species. The He(¹S)+Cl₂(³Π_u) interaction", *J. Chem. Phys.* **103**, 10116 - 10127 (1995).
8. S. M. Cybulski, R. Burcl, M. M. Szczyński and G. Chałasiński, "Ab initio study of the O₂(X³Σ_g⁻) + He(¹S) van der Waals cluster", *J. Chem. Phys.* **104**, 7997 - 8002 (1996).
9. A. Rohrbacher, J. Williams, K. C. Janda, S. M. Cybulski, R. Burcl, M. M. Szczyński, G. Chałasiński and N. Halberstadt, "Ab initio calculations of the interaction of He with the B³Π_{0u+} state of Cl₂ as a function of the Cl₂ internuclear separation.", *J. Chem. Phys.* **106**, 2685 - 2694 (1997).
10. R. Burcl, R. V. Krems, A. A. Buchachenko, M. M. Szczyński, G. Chałasiński and S. M. Cybulski, "RG + Cl(²P) (RG=He, Ne, Ar) interactions: Ab initio potentials and collision properties", *J. Chem. Phys.* **109**, 2144 - 2154 (1998).
11. J. Williams, A. Rohrbacher, J. Seong, N. Marianayagam, K. C. Janda, R. Burcl, M. M. Szczyński, G. Chałasiński, S. M. Cybulski and N. Halberstadt, "A three-dimensional potential energy surface for He (¹S) + Cl₂ (B³Π_{0u+}): *Ab initio* calculations and a multiproperty fit", *J. Chem. Phys.* **111**, 997 - 1007 (1999).
12. J. Kłos, G. Chałasiński, M. T. Berry, R. A. Kendall, R. Burcl, M. M. Szczyński and S. M. Cybulski, "*Ab initio* potential energy surface for the Ar(¹S) + OH(X²Π) interaction and bound rovibrational states", *J. Chem. Phys.* **112**, 4952 - 4958 (2000).
13. R. Burcl, P. Piecuch, V. Špirko, and O. Bludský, "Bound and quasi-bound states of the Li...FH van der Waals molecule", *Int. J. Quantum Chem. Symp.* **80**, 916-933 (2000).
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15. R. Burcl, R. D. Amos, N. C. Handy, "Study of excited states of furan and pyrrole by time-dependent density functional theory", *Chem. Phys. Lett.* **355**, 8-18 (2002).

- 16.** R. Burcl, P. Piecuch, V. Špirko, and O. Bludský, "Bound and quasi-bound states of the Li...FH van der Waals molecule: The effects of the potential energy surface and of the basis set superposition error", *J. Mol. Struct. (Theochem)* **591**, 151-174 (2002).
- 17.** R. Burcl, M. M. Szczęśniak, J. Klos, G. Chałasiński, and S. M. Cybulski, "*Ab initio* calculations and modeling of three-body forces in Ar₂H₂O", *Int. J. Quantum Chem.* **90**, 1215-1231 (2002).
- 18.** R. Burcl, N. C. Handy, and S. Carter, "Vibrational spectra of furan, pyrrole, and thiophene from a density functional theory anharmonic force field", *Spectrochim. Acta A*, **59**, 1881-1893 (2003).
- 19.** A. Caligiana, R. Burcl, N. C. Handy, D. P. Tew, and V. Aquilanti, "Anharmonic frequencies and Berry pseudorotation motion in PF₅", *Chem. Phys. Lett.*, **369**, 335-344 (2003).
- 20.** R. Burcl, S. Carter, and N. C. Handy, "On the representation of potential energy surfaces of polyatomic molecules in normal coordinates. II Parameterisation of the force field", *Chem. Phys. Lett.*, **373**, 357-365 (2003).
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- 22.** R. Burcl, S. Carter, and N. C. Handy, "Infrared intensities of furan, pyrrole, and thiophene: beyond the double harmonic approximation", *Chem. Phys. Phys. Chem.*, **6**, 340-343 (2004).