Graph Theoretic and Electronic Properties of Fullerenes

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Biasing Molecular Modelling Simulations with Experimental Residual Dipolar Couplings

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2015

A thesis presented in partial fulfilment of the
requirements for the degree of
Doctor of Philosophy
at
Massey University, Albany
New Zealand

Contents

Acknowledgements

There are several people I have to thank for making my last 3.5 years possible and enjoyable: Peter Schwerdtfeger, for giving me the opportunity to come to Massey University, and shielding all of us from the administrators. Thank you for support and a lot of freedom. · Jane Allison, for being extremely motivating, always taking time to answer and discuss my questions, and for the cake! · James Avery, for teaching me how to write less bad code, how to think and write as a mathematician (for chemists) and patience when either failed. Thank you for inviting me to stay in Copenhagen for two-and-a-half enjoyable and productive months. · Florian Senn and Lukáš Pašteka for useful discussions, advice, and encouragement when I was in need of it. · Andrew Punnett for taming the bits and electrons (as well as explaining how to) on smaller and larger computers, whenever and in whichever way they misbehaved. · Jayson Cosme, Lukáš Pašteka, and Lukas Trombach for the daily fix of ping pong (table tennis, to be accurate). · And everyone else in CTCP for the throughout friendly and encouraging atmosphere.

List of Publications

[1] Schwerdtfeger P, Wirz L, Avery J. Program fullerene: A software package for constructing and analyzing structures of regular fullerenes. *J Comput Chem* 2013, 34:1508–1526. doi:10.1002/jcc.23278.

[2] Wirz LN, Tonner R, Avery J, Schwerdtfeger P. Structure and properties of the nonface-spiral fullerenes T-C$_{380}$, D$_3$-C$_{384}$, D$_3$-C$_{440}$, and D$_3$-C$_{672}$ and their halma and leapfrog transforms. *J Chem Inf Model* 2014, 54:121–130. doi:10.1021/ci4005578.

[3] Schwerdtfeger P, Wirz LN, Avery J. The topology of fullerenes. *WIREs Comp Mol Sci* 2015, 5:96–145. doi:10.1002/wcms.1207.

[4] Wirz LN, Allison JR. Fitting alignment tensor components to experimental RDCs, CSAs and RQCs. *J Biomol NMR* 2015, 62:25–29. doi:10.1007/s10858-015-9907-x.

[5] Wirz LN, Tonner R, Hermann A, Sure R, Schwerdtfeger P. From small fullerenes to the graphene limit: A harmonic force-field method for fullerenes and a comparison to density functional calculations for Goldberg–Coxeter fullerenes up to C$_{980}$. *J Comput Chem* 2016, 37:10–17. doi:10.1002/jcc.23894.

[6] Wirz LN, Allison JR. Comment on "a tensor-free method for the structural and dynamic refinement of proteins using residual dipolar couplings". *J Phys Chem B* 2015, 119:8223–8224. doi:10.1021/acs.jpcb.5b02801.

[7] Wirz LN, Babić D, Avery J, Schwerdtfeger P. Toward tight upper and lower bounds for Hamilton cycles in fullerene graphs 2015.

[8] Sundholm D, Wirz LN, Schwerdtfeger P. Novel hollow all-carbon structures. *Nanoscale* 2015, 38:15886–15894. doi:10.1039/C5NR04370K.

Abstract

In this thesis two different models, that is levels of abstraction, are used to explore specific classes of molecular structures and their properties.

In part I, fullerenes and other all-carbon cages are investigated using graphs as a representation of their molecular structure. By this means the large isomer space, simple molecular properties as well as pure graph theoretical aspects of the underlying graphs are explored. Although chemical graphs are used to represent other classes of molecules, cavernous carbon molecules are particularly well suited for this level of abstraction due to their large number of isomers with only one atom type and uniform hybridisation throughout the molecule.

In part II, a force field for molecular dynamics, that is the step wise propagation of a molecular structure in time using Newtonian mechanics, is complemented by an additional term that takes into account residual dipolar couplings that are experimentally measured in NMR experiments. Adding this force term leads to more accurate simulated dynamics which is especially important for proteins whose functionality in many cases crucially depends on their dynamics. Large biomolecules are an example of chemical systems that are too large for treatment with quantum chemical methods but at the same time have an electronic structure that is simple enough for accurate simulations with a forcefield.