Synthetic, physical and computational chemistry of propeller-shaped polycyclic aromatic hydrocarbons

Ham, A. van der

List of Publications

1. van der Ham, A.,* Hansen, T.,* Lodder, G., Codée, J. D., Hamlin, T. A., & Filippov, D. V. (2019). Computational and NMR Studies on the Complexation of Lithium Ion to 8-Crown-4. *ChemPhysChem*, *20*(16), 2103-2109.

2. van der Ham, A., Schneider, G. F., & Lutz, M. (2021) CCDC 2056845: Experimental Crystal Structure Determination. doi: 10.5517/ccdc.csd.cc2719vg

3. van der Ham, A., Overkleeft, H. S., Schneider, G. F., & Filippov, D. V. (2021). A Three-step Synthesis of 4H-Cyclopenta[def]phenanthrene from Pyrene. *Eur. J. Org. Chem.*, 13, 2013-2017.

4. Arjmandi-Tash H., Bellunato, A., van der Ham, A., & Schneider, G. F. (2021). Inert Mask Lithography of Edge Narrowed Graphene Nanoribbons Directly Contacted to Metallic Electrodes. *Adv. Mater. Interfaces. 8*(20), 20100293.

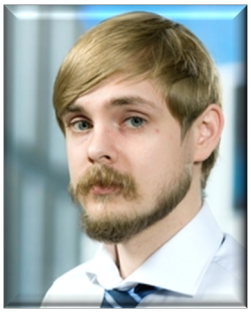
5. van der Ham, A.,* Liu, X.,* Calvani, D., Melcrová, A., Kozdra, M., Buda, F., Roos, W. H., Overkleeft, H. S., Filippov, D. V., & Schneider, G. F. (2021). Freestanding Non-covalent Thin Films of the Propeller-shaped Polycyclic Aromatic Hydrocarbon Decacyclene. *Manuscript accepted for publication in Nat. Comm.*

6. van der Ham, A.,* Hansen T.,* Filippov, D. V., Hamlin, T. A., & Scheider, G. F. (2021). Understanding the Conformational Preference of Propeller-shaped Polycyclic Aromatic Hydrocarbons Conformations. *Manuscript submitted. Available as pre-print at ChemRxiv* (doi: 10.26434/chemrxiv-2021-gfd9q)

7. van der Ham, A., Hansen, T., Brouwer A. M., Overkleeft, H. S., Hamlin, T. A., Filippov, D. V. & Schneider, G. F. (2021). Positional Effect of π-extension in Triple Helicenes. *Manuscript in preparation. Available as pre-print at ChemRxiv* (doi: 10.26434/chemrxiv-2021-kn2qg)

8. Crone, N. S. A., van Hilten, N., van der Ham, A., Boyle, A. L., Kros, A. Azobenzene-based amino acids for photocontrol of coiled coil peptides. *Manuscript in preparation.*

Curriculum vitae



Alex van der Ham was born on the 13th of March, 1993 in The Hague, The Netherlands. From 2005 until 2011 he attended the Adelbert College in Wassenaar where he obtained his secondary education diploma, with a specialization in the exact sciences (VWO). In his final year he participated in the 32nd National Chemistry Olympiad, becoming a top-10 finalist. Having both an interest in chemistry and cellular biology, in 2011 he started his Biopharmaceutical Sciences bachelor at the University of Leiden. As part of his Bachelors program he performed an internship at the Analytical Biosciences Department, under the supervision of dr. Peter Lindenburg. This research concerned the miniaturization of capillary electrophoresis (CE). He acquired his Bachelors' degree *cum laude* (ave. score > 85%) in 2014.

Having realized that chemistry was the greater of his passions, that same year he continued with a Masters' program in Medicinal chemistry, also at Leiden University. The first internship of one year was in the group of prof. dr. Mario van der Stelt, where he developed an *in vivo* active, nanomolar potent inhibitor for ABHD16a, an enzyme whose function at the time was still poorly understood. Where the desire was clear to continue a career in academia, for his second internship, he decided to develop his own research project. Under the supervision of dr. Dmitri Filippov, he synthesized the small crown ether 8C4, and investigated its binding to lithium ions using both NMR spectroscopy, as well as computationally, in collaboration with Thomas Hansen. This research would result in a paper, published in the journal ChemPhysChem. The Masters' degree, too, was obtained *cum laude*, in 2016.

After that he joined the group of dr. Grégory Schneider, with joined supervision by dr. Dmitri Filippov, with the goal of synthesizing and studying polycyclic aromatic hydrocarbons. In the five years that followed he would synthesize various aromatic molecules, including on a multigram scale, the results of which are concentrated in Chapter 2 of this Thesis. He studied these molecules with a wide range of analytical techniques, ranging from spectroscopic techniques like IR, Raman, UV-Vis and NMR, to microscopic techniques like SEM, TEM and AFM, the fruits of which are found in Chapters 3 and 5. Moreover, the computational work that started at the end of his Masters would prove to be the starting point for a fond interest in computational chemistry, the results of which are scattered throughout this Thesis, but are primarily located in Chapter 4.

Parts of the work reported in this thesis were presented in the form of a poster both on national (CHAINS 2016 – 2020; Reedijk Symposium 2017 – 2019) and

international conferences (Chem2DMat 2017 (Strassbourg) and 2019 (Dresden); Nobel Prize Conference 2018 (Groningen)). A poster prize was obtained at the Reedijk Symposium in 2019. He also gave an oral presentation on his work at CHAINS 2020.

His broad interests, already evidenced in his early years, made him now pursue a post-doctoral position in NMR spectroscopy in the United Kingdom, particularly in the groups of prof. dr. Gareth A. Morris in Manchester, and that of prof. dr. Simon B. Duckett at the University of York.

Acknowledgments

A PhD is never a lone man's journey. Faces come, faces go, and each encounter shapes you. As such, I would like to start by thanking my two co-promotors, Grégory and Dima, who helped me in becoming the scientist I am today.

I would like to thank Thomas, not only for being a mentor and guide into the field of computational chemistry, but also a respected colleague and kind friend. The same goes for Xue, who has been my office mate for almost the entire duration of my PhD and whose expertise in the material science field has been invaluable when it comes to experimental work and publications. The second long term office mate to especially mention is Pauline, with whom I shared many a banter moment, on both scientific as well as (well, mostly) non-scientific topics.

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This list would not be complete without also thanking Fons and Karthick for the many hours invested in making the crazy NMR experiments I kept throwing at them actually happen, and helping me prepare for my future in NMR spectroscopy. Similarly, I would like to thank Dario for the nice and fruitful collaborations. And a final thankyou goes to all the others from Biosyn and SBC, with whom I collaborated, or who were simply able to put a smile on my face.

I would like to conclude by thanking Anna, without whom my PhD, indeed my life, would not have been the same!

Alex