Appendix File Guide

The following information serve as a guide for finding and reading the relevant supplementary data supporting the findings of this thesis.

Contents of the Appendix

The Appendix is composed of three file formats:

1. **Computational chemistry output files**, that are read as the graphical files of the computed, in the thesis, molecular/supramolecular structures. The output/graphical files, for visualizing the structures, are collected in the respective '**A***x*-**G***x*' folders (where the '*x*' suffix denotes the corresponding Chapter number).
2. **MS Excel files**, that contain the detailed tables with all numerical data of computed and processed energy data, the molecular geometry information, as well as their corresponding plots.
3. And two pdf **documents**: this file guide, and a document with the remaining experimental details.

- **Computational Chemistry Files**

Due to the size and complexity of the supramolecular structures computed in this thesis their image and visualisation is provided as graphical type files. These can be visualized in a three-dimensional setup with available rotation and translation of the structure. There are over 150 computed geometries in this work, therefore use of selected graphical files is 'economically' sensible for the examination of these structures.

Three computational methods were used for optimising the molecules studied in this work: The PMx (PM6, PM6-D3H4X, PM7) Hamiltonians, GFN2-xTB and a DFT method B3LYP (with Gaussian09). The PMx output files, that concern mainly Chapter 4 (with two structures also found in Chapter 5), are available via the **.out* type files, named appropriately with the method indicated in the filename (where '*' is the wildcard character denoting any given filename that accompanies a given file extension where noted). Similarly, the GFN2-xTB graphical output can be opened via the **xtbopt.xyz* type files.

Additional conformational analysis computations, are provided via a CREST output graphical file the 'A6d_(Ch.6.4_crest_conformers).xyz' file, provides an animation file containing all the coordinates for all conformers found in A6_G6 (viewed with Avogadro 1.02). Finally, two **.gif* animations are provided to show the formation of the seed dimers of Chapter 5.3.1 in the A5_G5 graphical folder.

Opening and reading the graphical content of these file types can be done directly with the open source **Avogadro 1.02** program (download at https://avogadro.en.softonic.com/). Other software such as Jmol, Molden 2.0 or GaussView can be used according to preference or availability, amongst other available programs that similarly serve this purpose. Specific assignment of the filenames to their corresponding structure and numerical information is detailed in the relevant MS Excel files.

- ## MS Excel Files

The MS Excel **.xlsx* files , named as **A***x*.xlsx (with *'x'* suffix denoting the relevant Chapter number), contain all the computational optimisation energy data. The computational chemistry file names are assigned to each structure clearly therein. All the raw collected and processed numerical data of the ground state energies, their binding energies and the geometrical details (angles, bond lengths, intermolecular 'slippage' θ), as well as corresponding plots are contained in these MS Excel files.

- **Documents**

The presented here '*Appendix_file_guide*' document is one of the two pdf documents found in the Appendix. The other pdf document '*A5-S*' details the complementary spectroscopic and experimental data provided by the experimentalist collaborators, concerning the Chapter 5.3.1 content.