## README – Raw Data Upload for the Article

# "Unlocking twofold oxidation in phenothiazine polymers for application in symmetric all-organic anionic batteries"

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Raw Data for the various analytical methods and calculations is compressed into one .zip file each for every method.

- Nuclear Magnetic Resonance (NMR)
  - Raw Data for each compound (readable with BRUKER TopSpin, MESTRELAB MestReNova)
- Mass Spectroscopy (MS)
  - .xy file + raw data file for each compound OR .docx file with image of the spectrum
- Gel Permeation Chromatography (GPC)
  - .txt files containing elugram and molecular weight distribution data
  - .pdf sample report
- Infrared Spectroscopy (IR)
  - .txt files
- Ultraviolet and Visible Light Spectroscopy (UV/Vis)
  - .txt files
- Thermogravimetric Analysis (TGA)
  - .txt files
- Differential Scanning Calorimetry (DSC)
  - .txt files
- Composition and Masses of Electrodes
  - .xlsx file including the weigh-in for all components, as well as the weights of all electrodes and blank cut-outs.
- Electrochemical Measurements in Solution
  - .txt files for the measurement and for the reference *vs.* $Fc/Fc^+$
- Electrochemical Measurements in Swagelok-type Battery Cells
  - .xlsx file with all electrode masses. Divided into separate electrode films from which the electrodes have been cut out. The composition of each of those films is also given
  - All electrochemical measurements are sorted by the figure in which they are presented. Multiple figures may be based on the same measurement. The film and electrode used in each measurement can be taken from the metadata in the file name of the respective raw data. Nomenclature is: RW-Bxx_yy_zzz… (xx: number of the film, yy: number of the electrode, zzz: additional information about measurement parameters.)
  - Each measurement consists of:
    - .mps files containing the settings for the measurements procedure as taken from the respective biologic potentiostats (readable by text editor). These settings files often contain additional procedures neither discussed in the manuscript nor the ESI. Metadata such as characteristic masses, reference electrodes etc. contained in the .mps files are default settings and do not represent reality. .mps files are solely included to provide access to the measurement techniques / procedures.

        - .mpr files containing the raw data (only readable by EC-Lab Software by BIOLOGIC).
        - .txt files with exported raw data containing all measured and parameters calculated by the analysis software.
- Density Functional Theory (DFT) Calculations
    - coord.xyz coordinates files of the optimized structure used as input for the single point calculations, as well as the NICS-calculations.
    - ridft.out output file of the TURBOMOLE RIDFT-calculations. Orbital energies and the occupation can be found here.
    - xx.cub files for Calculated Orbitals on cubic 3D-grid. The File-Name gives the number of the orbital.
    - td.plt and tp.plt files for plotting the total electron density and electrostatic potential (only calculated for the dicatons, used for the electrostatic potential maps).
    - sd.plt file for plotting the spin density.
    - xx-allcenter.armdat output-File of the AROMA-script. The NICS(ZZ) is the oop (out-of-plane)-column.
- Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray spectroscopy (EDX)
    - .tif files