

# Readme - Dataset to "Between Order and Confusion: Clearing Up Structural Misconceptions in Carbon Materials Nomenclature"

## Purpose of the data collection:

The publication "Between Order and Confusion: Clearing Up Structural Misconceptions in Carbon Materials Nomenclature" compares the structural characteristics of different graphene-containing carbon materials, namely graphite, graphitic carbon, non-graphitic carbon and amorphous carbon. As the nomenclature by the International Union of Pure and Applied Chemistry (IUPAC) is based on these structural characteristics, the importance of a consistent characterization and description of these carbon materials is stressed in order to prevent misutilization of terminology and miscommunication between scientists. To do so, X-ray diffraction and Raman Spectroscopy serve as main analytical methods to underline and investigate structural differences. As X-ray scattering data and Raman spectra graphitic and non-graphitic carbons are already published in previous works, they have been reprinted in the above-mentioned publication. To complete the data materials comparison, X-ray scattering data and Raman spectra of graphite and an amorphous Kraft-Lignin carbon sample have been collected in addition, which presents the data that is provided here.

## Details about materials:

- Graphite, graphite flakes, 99%, carbon basis, -325 mesh particle size (50 – 70%), Sigma-Aldrich
- Cleaved Kraft-Lignin extracted from spruce and pine wood, Fraunhofer Center for Chemical-Biotechnological Processes (CBP), Leuna, Germany

## Details about data acquisition:

X-ray scattering data of both samples (graphite and amorphous Kraft-Lignin) were collected with a XRDynamic 500 diffractometer from Anton Paar in Bragg-Brentano geometry at room temperature. Cu-K<sub>α1</sub> radiation ( $\lambda = 1.5406 \text{ \AA}$ ) and Cu-K<sub>α2</sub> radiation ( $\lambda = 1.5444 \text{ \AA}$ ) in a 1:2 ratio were applied with a current of 50 mA and a voltage of 40 kV. Measurement was done in the range of  $10^\circ < 2\theta < 115^\circ$  with a step size of  $0.05^\circ$  for graphite and a step size of  $0.1^\circ$  for the amorphous Kraft-Lignin sample. Measurements were carried out by Chantal Glatthaar (Institute of Physical Chemistry, Justus Liebig University, Gießen, Germany) in June 2025.

A Renishaw inVia Raman microscope system in backscattering geometry was used at room temperature with a 50 x objective to generate Raman spectra of both samples. For graphite, the laser power was 5 mW, the laser excitation wavelength was  $\lambda = 515 \text{ nm}$ , the spectral range was  $100 - 3200 \text{ cm}^{-1}$  and 5 accumulations of 10 s were the integral exposure time. In case of amorphous Kraft-Lignin, the laser power was 5 mW, the laser excitation wavelength was  $\lambda = 633 \text{ nm}$ , the spectral range was  $150 - 4000 \text{ cm}^{-1}$  and 4 accumulations of 10 s were the integral exposure time. Measurements were carried out by Limei Chen (Institute of Experimental Physics I, Justus Liebig University, Gießen, Germany) in June 2025. Auto-fluorescence of lignin causes an intense fluorescent background. Hence, a baseline was created and the background subtracted to obtain a representative Raman spectrum for amorphous carbon. Each contribution (experimental data, baseline and corrected data by background subtraction) is included in the respective file of Raman data for Kraft-Lignin amorphous carbon.

## Structure of provided data:

In sum, four files are part of this data set. For each measurement a new file was created. The name of the .txt file clearly indicates the data that are stored in the respective file. X-ray scattering data of graphite is provided in "XRD Data Graphite.txt" and X-ray scattering data of amorphous Kraft-Lignin is given in "XRD Data for Kraft-Lignin Amorphous Carbon.txt". Raman spectroscopy data for graphite is provided in "Raman Data Graphite.txt" and Raman spectroscopy data for amorphous Kraft-Lignin is given in "Raman Data for Kraft-Lignin Amorphous Carbon.txt". Measured variable, intensity and respective units are provided in each file in order that re-usage and plotting of this data is unambiguous for everyone.