# Molecules

ID, group, name, Summenformel, molecular formula (image/ChemDraw), SMILES-String

## Single Molecules

ID, *further information*

## Triplet-Doublet pairs

ID, Doublet, Linker, Chromophore

(Linker includes possibility to define bimolecular systems and supramolecular systems)

## Radical pairs

ID, Radical 1, Radical 2

## Triplet-Triplet pairs

ID, Triplet 1, Triplet 2

# Measurement

ID, Molecule, Method, Temperature, Solvent, *Concentration*, Date, *Location*, *Device*, *Series*, Path to the dataset, data corrected? Data evaluated?

## TREPR

ID, Frequency (XQW), Excitation wavelength, *Excitation energy*, Attenuation, *Number of scans*, *Repetition rate, Mode*

## CWEPR

ID, Frequenz (XQW), Attenuation

## UVVIS

ID, Dimension of the cuvette

## Fluorescence

ID, Excitation or emission?, Wavelength, OD (Absorbance)

## FS-TA

ID, Excitation wavelength, Excitation energy

## NS-TA

ID, Excitation wavelength, Excitation energy

## NMR

ID, Frequency

## QY

ID, Excitation wavelength

## SPT

ID, Excitation wavelength, Filter

## PULSE EPR (TN, PEANUT, PELDOR, saturation recovery...)

ID, Type (e.g. PEANUT, PELDOR…), Path to DSC-File