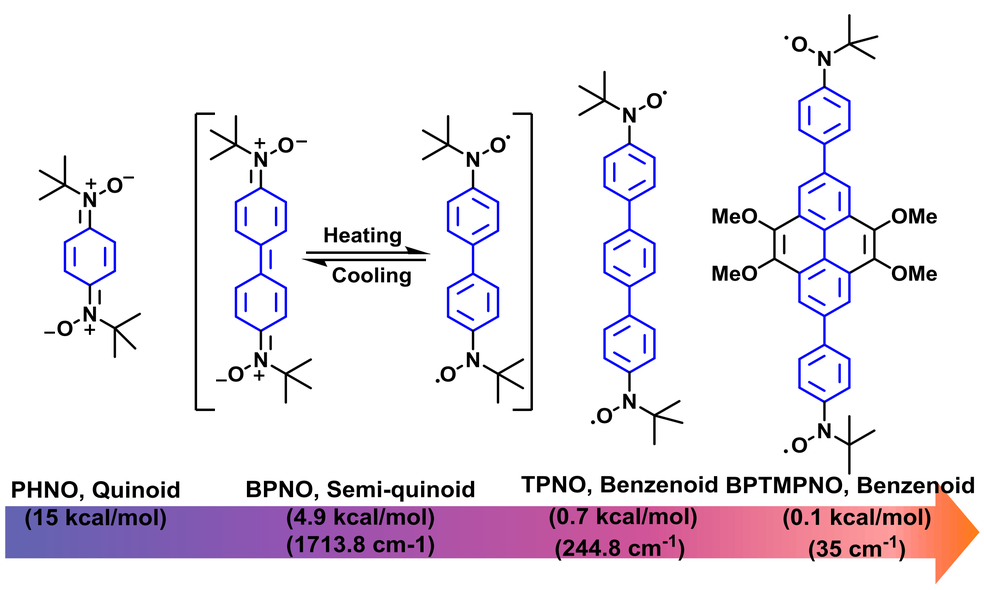
B5 Rational design with input from DFT calculations and preparation of coordination polymer-based quantum magnets

Martin Baumgarten (MPI-P Mainz)

Varifying bis(tert-butylnitroxide)s

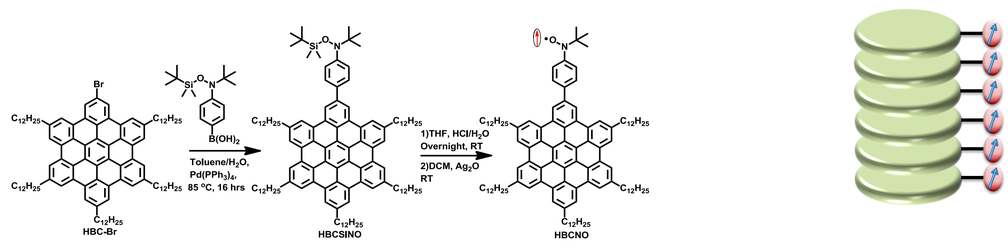


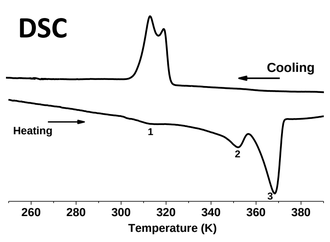
For BPNO similar strong coupling as for TMPNO – semiquinoid structure.
Biradical features only at elevated temperatures.
For TPNO and BPTMPNO typical biradical forms, where the intramolecular exchange can be further fine tuned by substituents.

Ravat, Baumgarten *PCCP* **17**, 983-991 (2015)

HBC derivatives

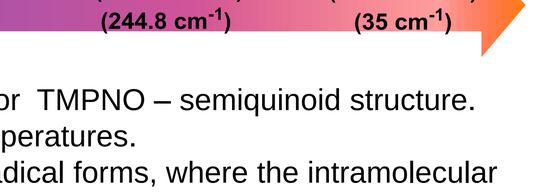
A spin bearing hexabenzocorone (HBC), biradicals so far not available



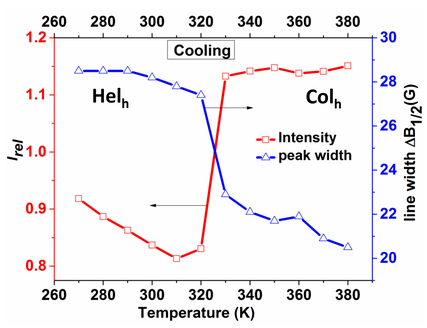


Helical hexagonal (T<300 K) –
Columnar hexagonal (T> 370 K)

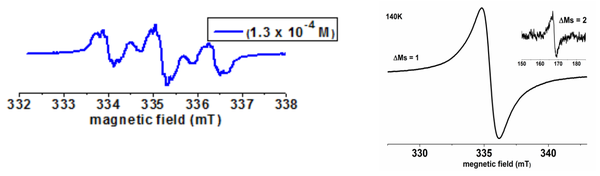
2D-WAXS at 255 K



Positive Magneto LC effect



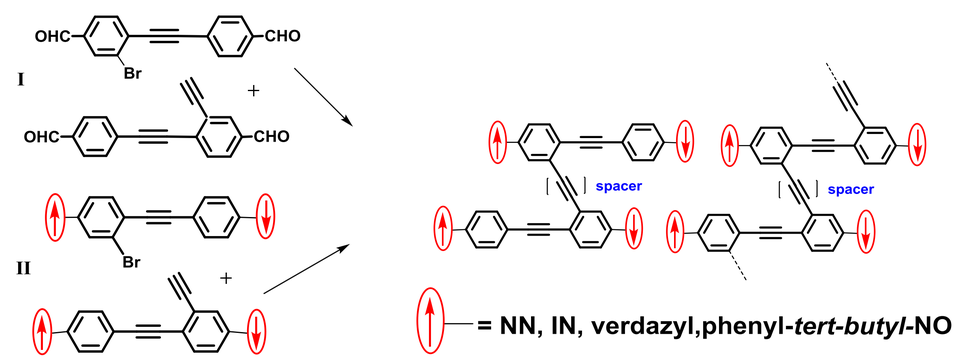
Intermolecular induced biradical features EPR spectra



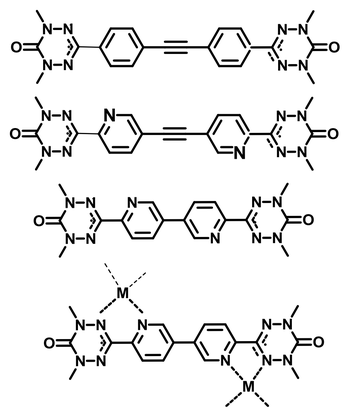
Ravat et al. *J. Am. Chem. Soc.* **136**, 12860-3 (2014

Project goals and work program

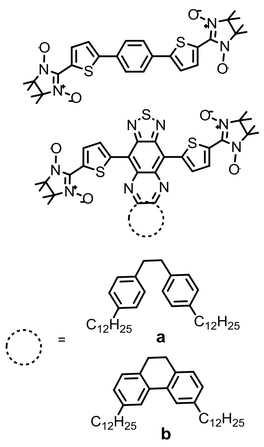
Covalently linked biradicals, two synthetic pathways



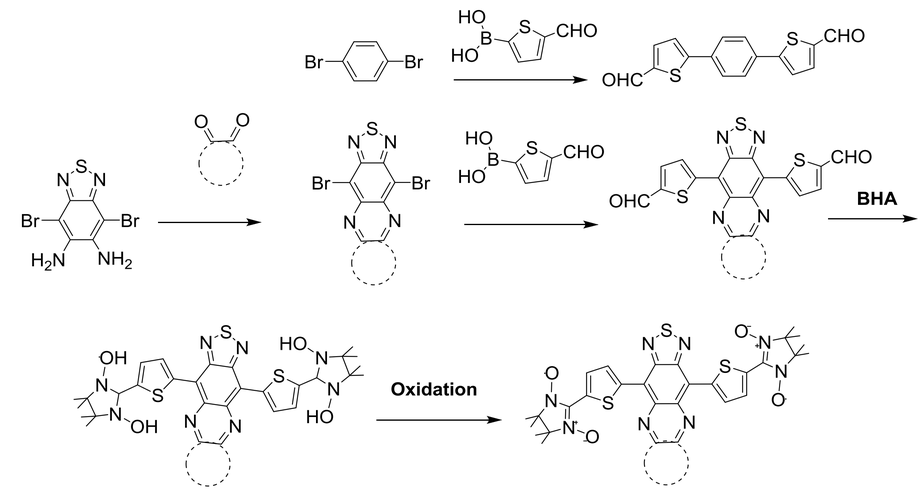
Verdazyls with additional ligation site



Varying donor/acceptor strength of the bridge



Example of multistep Synthesis



According to
An et al. Chem. Mater. **26**, 5923 (2014)

Role within the TR49

- **Providing new 2d and 3D ordered biradicals arranged via self-organization as hydrogen bonding, metal complexation, or even covalently controlled interdimer exchange.**

B1 **magnetic characterizations of suitable crystals by SQUID and AC susceptibility, turther thermal expansion.**

B2 **B3** **in depth ab initio DFT calculations for magnetic coupling pathways and Quantum Monte Carlo simulations for analysis of dimensionality.**

Staff requested

- **N.N. (Ph.D. student) (auxiliary support)**

- Synthesis of extended biradicals.

- For teaching and learning the optimization of experimental conditions, some former biradicals may be upscaled and crystallized.

- Full characterization of samples along the list of methods.

Methods

Organic Synthesis and standard structural analysis (Mass, NMR, ..).

Crystal Growth:

X-ray crystal structure analysis:

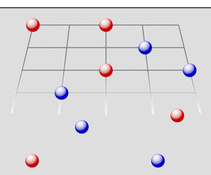
DFT calculations of discrete biradicals and next neighbor interactions:

UV-Vis absorption studies of defined biradicals:

EPR spectroscopic studies:

Magnetization measurements, AC susceptiblities : **B1**

QMC and ab initio modelling in correlated antiferromagnets: **B2** **B3**



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