

# Polymorphism in *P,P*-[3]ferrocenophanes: Insights from an NMR crystallographic approach

## -Supplemental Materials Section-

Thomas Wiegand<sup>[a]#</sup>, David Lüdeker<sup>[a]#</sup>, Gunther Brunklaus,<sup>[a]\*</sup>, Kathrin Bussmann<sup>[b]</sup>, Gerald Kehr<sup>[b]</sup>, Gerhard Erker,<sup>[b]\*</sup> and Hellmut Eckert<sup>[a]\*</sup>

<sup>[a]</sup> Dr. Thomas Wiegand, MSc David Lüdeker, PD Dr. Gunther Brunklaus, Prof. Dr. Hellmut Eckert

Institut für Physikalische Chemie and Graduate School of Chemistry, WWU Münster

Corrensstrasse 30, D 48149 Münster, Germany

Fax: (+49)-251-83-29159

E-Mail: [eckerth@uni-muenster.de](mailto:eckerth@uni-muenster.de)  
[gbrunklaus@uni-muenster.de](mailto:gbrunklaus@uni-muenster.de)

<sup>[b]</sup>Kathrin Bussmann, Dr. Gerald Kehr, Prof. Dr. Gerhard Erker

Organisch-Chemisches Institut, WWU Münster

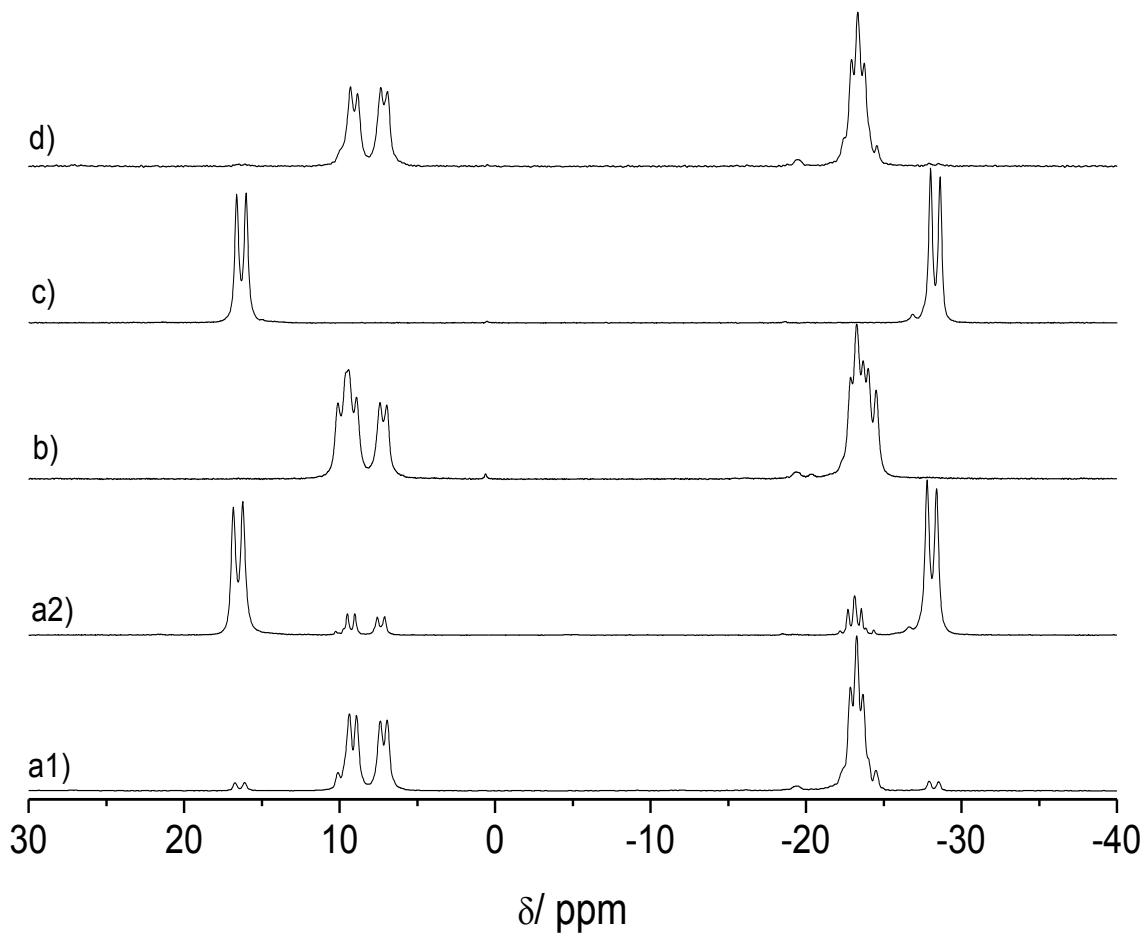
Corrensstrasse 40, D 48149 Münster, Germany

Fax: +49-251-83-36503

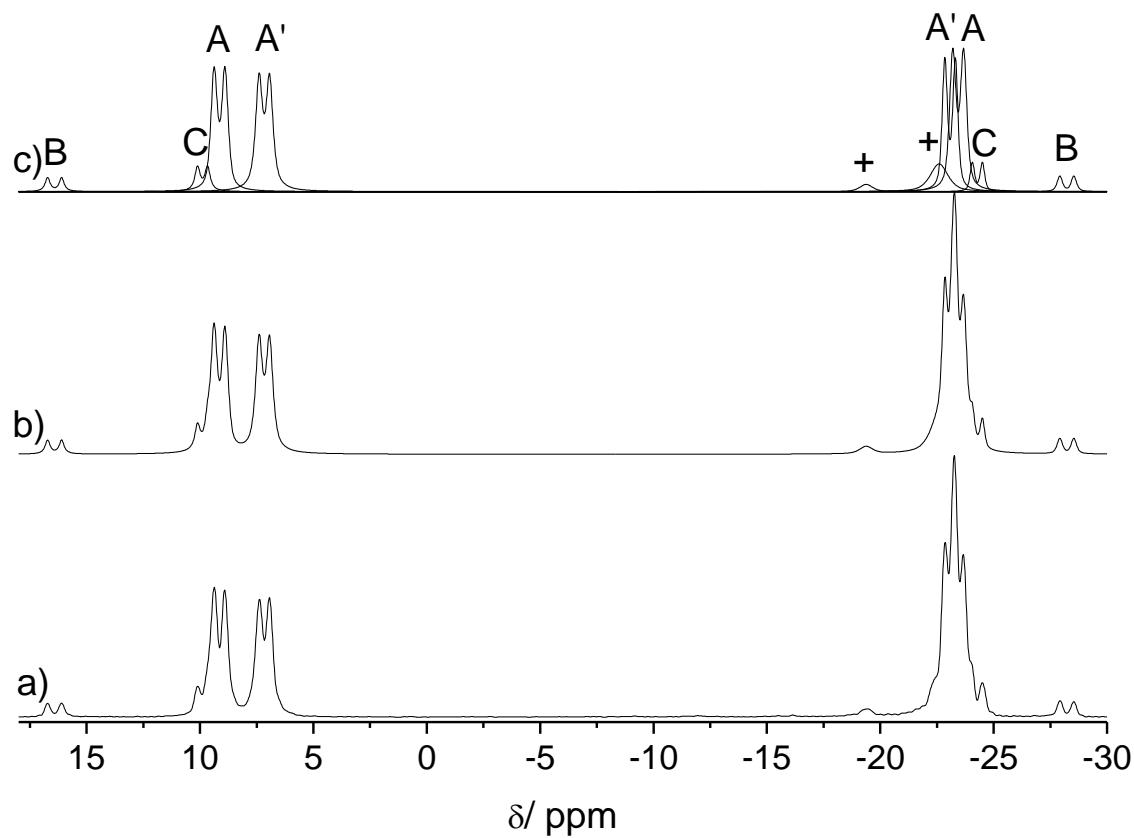
E-Mail: [erker@uni-muenster.de](mailto:erker@uni-muenster.de)

#: Both authors contributed equally.

\*: Corresponding authors.



**Figure S1:**  $^{31}\text{P}\{\text{H}\}$  CPMAS-NMR spectra of **1** (rac.)- $\text{C}_{38}\text{H}_{46}\text{FeP}_2$ . (a1) Slowly crystallized sample ( $2^{\text{nd}}$  preparation series), (a2) solvent removed at vacuum ( $2^{\text{nd}}$  preparation series), (b) Sample obtained by slow crystallization over several days ( $1^{\text{st}}$  preparation series), (c) same sample measured after 2 months and (d) same sampled stored for one week in a desiccator over dichloromethane.



**Figure S2:** Solid State  $^{31}\text{P}\{\text{H}\}$  CPMAS NMR spectrum of a slowly crystallized sample of 1-rac- $\text{C}_{38}\text{H}_{46}\text{FeP}_2$  and its corresponding spectral deconvolution into the distinct contributions from polymorphs A, B, and C.