

Supplementary Material

The pentanuclear Fe^{II} cluster [(C₅H₄)₆Fe₅]²⁻ - bringing together ferrocene sandwiches and homoleptic Fe^{II}-cyclopentadienyl σ -complexes.

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Details of the X-ray crystal structure analysis of 1 and 2:

Crystals of **1** and **2** were selected and mounted in an inert oil and transferred to the cold gas stream of the diffractometer. For both compounds, data collection was performed on a Stoe IPDS-II two circle diffractometer with graphite-monochromated Mo- K_{α} radiation. An empirical absorption correction with the MULABS option¹ in the program PLATON² was performed. Equivalent reflections were averaged. The structure was solved by direct methods³ and refined with full-matrix least-squares on F^2 using the program SHELXL-97⁴. Hydrogen atoms were placed on ideal positions and refined with fixed isotropic displacement parameters using a riding model.

The differing atoms in **1** and **2** could be unequivocally determined. They showed up in a difference map with clearly distinguishable heights and could be successfully refinement as Li in **1** and Fe in **2**. It is impossible to refine Li(2) and Li(3) as Fe in **1** and Fe(3) as Li in **2**.

- 1 R. H. Blessing, *Acta Crystallogr. Sect. A.*, 1995, **51**, 33.
- 2 A. L. Spek, *Acta Crystallogr. Sect. A.*, 1990, **46**, C34.
- 3 G. M. Sheldrick, *Acta Crystallogr. Sect. A.*, **1990**, 46, 467.
- 4 G. M. Sheldrick, *SHELXL-97. A Program for the Refinement of Crystal Structures*, Universität Göttingen, 1997.

Crystal data of 1 determined at T = 173 K: $C_{42}H_{56}Fe_3Li_6N_4$, $M = 826.10 \text{ g mol}^{-1}$, monoclinic, $a = 21.420(5) \text{ \AA}$, $b = 10.730(3) \text{ \AA}$, $c = 17.830(4) \text{ \AA}$, $\beta = 99.533(17)^{\circ}$, $U = 4041.4(17) \text{ \AA}^3$, $T = 173(2) \text{ K}$, space group $C2/c$, $Z = 4$, $\mu(\text{Mo-}K_{\alpha}) = 1.097 \text{ mm}^{-1}$, 9280 reflections measured, 3787 unique ($R_{\text{int}} = 0.1753$) which were used in all calculations. The final $wR(F^2)$ was 0.1055 (all data).

Figure 1S: Crystal structure of compound **1**; thermal ellipsoids shown at the 50% probability level.

