Supplementary Material

The pentanuclear Fe\textsuperscript{II} cluster [(C\textsubscript{5}H\textsubscript{4})\textsubscript{6}Fe\textsubscript{5}]\textsuperscript{2-} - bringing together ferrocene sandwiches and homoleptic Fe\textsuperscript{II}-cyclopentadienyl $\sigma$-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$_\alpha$ radiation. An empirical absorption correction with the MULABS option$^1$ in the program PLATON$^2$ was performed. Equivalent reflections were averaged. The structure was solved by direct methods$^3$ and refined with full-matrix least-squares on $F^2$ using the program SHELXL-97$^4$. 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.


Crystal data of 1 determined at T = 173 K: C$_{42}$H$_{56}$Fe$_3$Li$_6$N$_4$, $M = 826.10$ g mol$^{-1}$, monoclinic, $a = 21.420(5)$ Å, $b = 10.730(3)$ Å, $c = 17.830(4)$ Å, $\beta = 99.533(17)^\circ$, $U = 4041.4(17)$ Å$^3$, $T = 173(2)$ K, space group C2/c, $Z = 4$, $\mu$(Mo-K$_\alpha$) = 1.097 mm$^{-1}$, 9280 reflections measured, 3787 unique ($R$$_{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.