

Supplementary Material

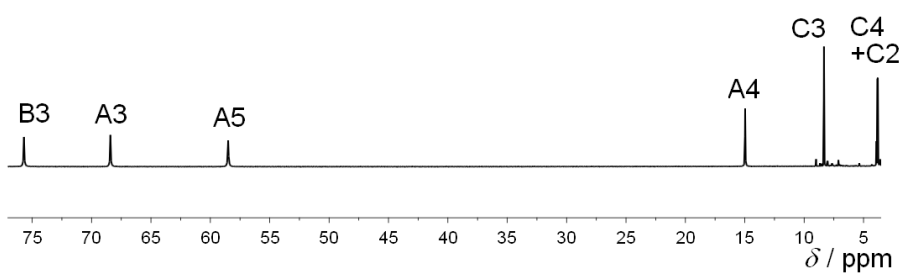


Fig. S1 Part of the 600 MHz  $^1\text{H}$  NMR spectrum of a  $(\text{CD}_3)_2\text{CO}$  solution of  $[\text{Fe}(\mathbf{2})_2][\text{PF}_6]_2$  at 295 K.

Table S1:

Comparison of Fe–H distances from X-ray diffraction ( $d1$ - $d4$ ) and PRE

#	$d1/\text{\AA}$	$d2/\text{\AA}$	$d3/\text{\AA}$	$d4/\text{\AA}$	$d_{av}/\text{\AA}$	$d_{calc}/\text{\AA}$	$Iw_{exp}/\text{Hz}$
D2	3.57	3.07	3.06	3.70	3.35	3.65	1440
D3	4.66	5.24	4.63	5.32	4.96	5.16	180
D5	5.92	6.35	6.02	6.27	6.14	5.79	90
D6	4.83	5.11	4.93	4.94	4.95	5.03	210
A3	4.99	5.03	5.04	4.94	5.00	4.99	220
A4	5.87	5.87	5.92	5.82	5.87	5.79	90
A5	5.33	5.19	5.25	5.30	5.27	5.03	210
B3	5.04	5.01	5.02	5.00	5.02	5.03	210