

Synthesis, Spectral Characterization, and Structural Modelling of Di- and Trinuclear Iron(III) Monensinates with Different Bridging Patterns

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Supporting information

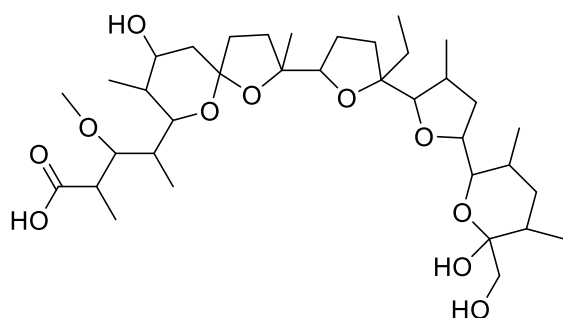


Figure S1. Structure of monensin.

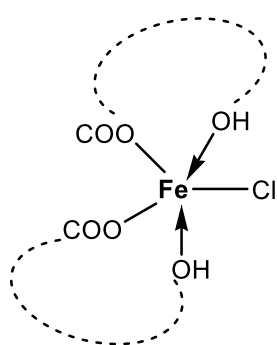


Figure S2. Proposed structure of mono-complex **1a**.

Table S1. ^{13}C -NMR chemical shift (δ , ppm) of monensic acid and complex **1** in CDCl_3 ($\Delta = \delta_1 - \delta_{\text{MonH}}$).

Carbon	MonH \times H $_2$ O	1	Δ		Carbon	MonH \times H $_2$ O	1	Δ
1	177.6	177.4	-0.2		19	32.8	32.7	-0.1
2	42.3	42.2	-0.1		20	77.4	77.3	-0.1
3	81.8	81.7	-0.1		21	74.0	73.9	-0.1
4	36.9	36.8	-0.1		22	33.1	33.0	-0.1
5	67.3	67.1	-0.2		23	36.9	36.8	-0.1
6	34.8	34.7	-0.1		24	35.8	35.7	-0.1
7	70.9	70.8	-0.1		25	97.5	97.3	-0.2
8	34.4	34.3	-0.1		26	68.1	68.0	-0.1
9	108.1	108.0	-0.1		27	15.9	15.9	0.0
10	38.6	38.5	-0.1		28	58.3	58.2	-0.1
11	34.0	33.9	-0.1		29	10.6	10.5	-0.1
12	85.4	85.3	-0.1		30	11.0	10.9	-0.1
13	83.7	83.6	-0.1		31	28.1	27.9	-0.2
14	28.0	27.9	-0.1		32	31.4	31.3	-0.1
15	31.8	31.7	-0.1		33	8.8	8.7	-0.1
16	86.8	86.6	-0.2		34	16.0	15.8	-0.2
17	85.1	85.0	-0.1		35	17.8	17.7	-0.1
18	34.6	34.6	0.0		36	16.7	16.6	-0.1

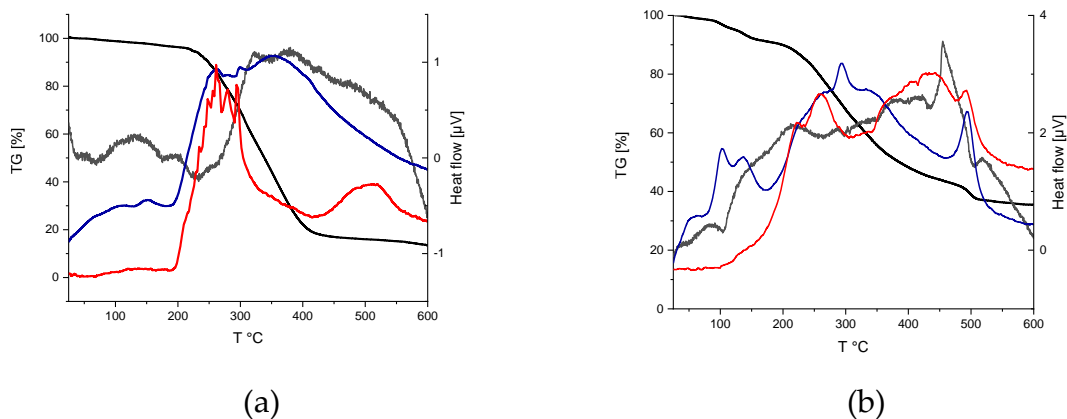


Figure S3. TG-DTA/MS curves of (a) complex 1 and (b) complex 2.

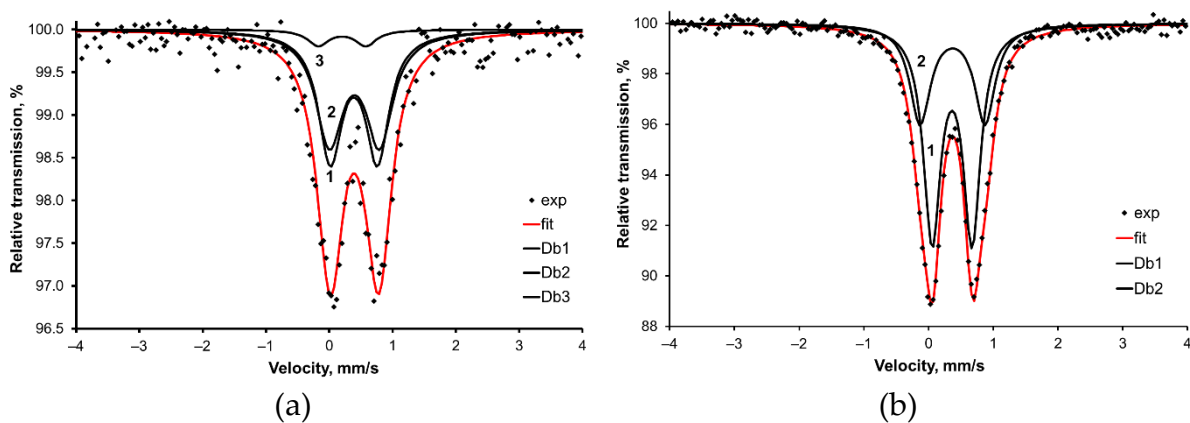
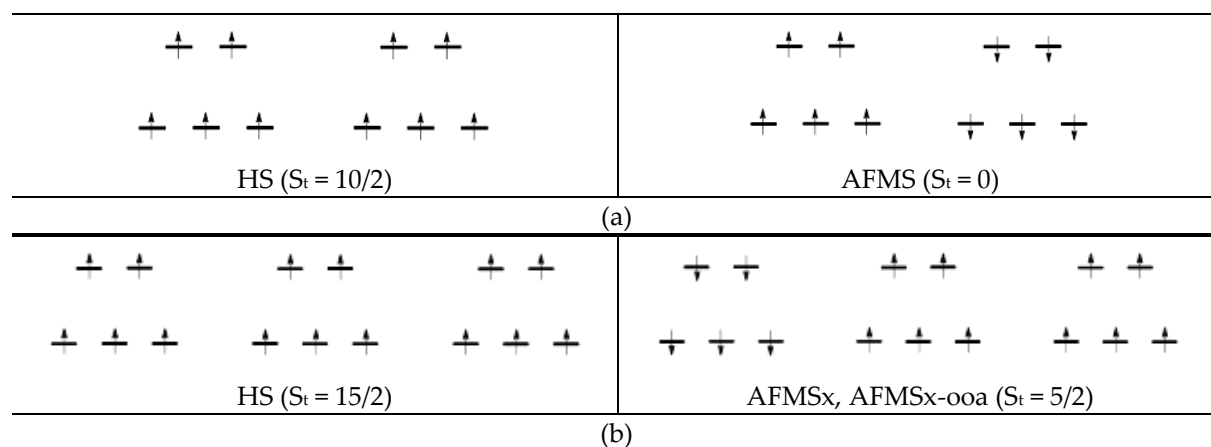


Figure S4. Mössbauer spectra at 77 K: (a) complex 1, (b) complex 2.



Scheme S1. Electron configurations of the iron ions in (a) complex 1 and (b) complexes 2.