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Supplementary material

SUPPLEMENTARY MATERIAL TO

Solution behaviour of (*N*,*N′*-ethylenebis(salicylideneiminato))-iron(III) chloride in aqueous methanol at 298.15, 303.15 and 313.15 K

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TABLE S-I. Densities (ρ) and viscosities (η) of different aqueous methanol solutions at different temperatures; w_1 – mass fraction of methanol

w_1	T / K	$\rho\times10^{-3}$ / kg m^{-3}		η / mPa s	
		Exp.	Lit.	Exp.	Lit.
1.00	298.15	0.78662	0.78645[1]	0.5469	0.542[1]
	303.15	0.78188	0.7819[2]	0.5092	0.510[2]
	313.15	0.77280	0.7720[3]	0.4488	0.4470[3]
0.90	298.15	0.81582	0.8158[4]	0.7619	0.7885[4]
	303.15	0.81084	0.8108[4]	0.7112	–
	313.15	0.80236	0.8023[4]	0.6344	–
0.80	298.15	0.84237	0.8424[4]	1.0036	1.0241[4]
	303.15	0.83769	0.8378[4]	0.9634	–
	313.15	0.82961	0.8294[4]	0.8871	–
0.70	298.15	0.86761	0.8675[4]	1.1849	1.2335[4]
	303.15	0.86310	0.8630[4]	1.1430	–
	313.15	0.85532	0.8550[4]	1.0620	–
0.60	298.15	0.89113	0.8910[4]	1.4091	1.4264[4]
	303.15	0.88649	0.8864[4]	1.3689	–
	313.15	0.87885	0.8787[4]	1.3017	–

TABLE S-II. Molalities (m), densities (ρ), viscosities (η), and apparent molar volumes (φ_V) of Fe^{III}(salen)Cl in different aqueous methanol solutions at different temperatures; w_1 – mass fraction of methanol

m / mol kg^{-1}	$\rho\times10^{-3}$ / kg m^{-3}	η / mPa s	$\varphi_V\times10^6$/m^3 mol^{-1}
w_1 = 1.00			
T = 298.15 K			
0.0025	0.78706	0.5539	170.12
0.0036	0.78728	0.5575	158.24

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TABLE S-II. Continued

m / mol kg^{-1}	ρ×10^{-3} / kg m^{-3}	η / mPa s	φ_V × 10^6/m^3 mol^{-1}
	w_1 = 1.00		
	T = 298.15 K		
0.0056	0.78774	0.5638	131.25
0.0076	0.78825	0.5710	107.82
0.0097	0.78876	0.5781	97.84
0.0117	0.78931	0.5879	82.80
	T = 303.15 K		
0.0025	0.78234	0.5164	156.34
0.0036	0.78256	0.5209	148.30
0.0056	0.78302	0.5272	124.24
0.0076	0.78353	0.5327	102.06
0.0097	0.78405	0.5399	91.22
0.0117	0.78459	0.5472	78.26
	T = 313.15 K		
0.0025	0.77327	0.4551	147.90
0.0036	0.77349	0.4595	141.73
0.0056	0.77397	0.4650	112.78
0.0076	0.77446	0.4705	96.85
0.0097	0.77498	0.4761	86.23
0.0117	0.77552	0.4815	73.26
	w_1 = 0.90		
	T = 298.15 K		
0.0025	0.81625	0.7659	179.86
0.0034	0.81646	0.7697	155.44
0.0054	0.81692	0.7772	132.14
0.0074	0.81741	0.7884	115.32
0.0093	0.81794	0.7961	95.63
0.0113	0.81849	0.8055	83.10
	T = 303.15 K		
0.0025	0.81129	0.7151	167.20
0.0034	0.81149	0.7189	150.17
0.0054	0.81195	0.7246	128.25
0.0074	0.81244	0.7321	111.99
0.0093	0.81298	0.7415	90.84
0.0113	0.81353	0.7509	78.73
	T = 313.15 K		
0.0025	0.80282	0.6383	159.83
0.0034	0.80303	0.6428	139.52
0.0054	0.80350	0.6494	117.64
0.0074	0.80399	0.6559	103.37
0.0093	0.80453	0.6625	83.07
0.0113	0.80508	0.6692	71.60

TABLE S-II. Continued

m / mol kg^{-1}	ρ×10^{-3} / kg m^{-3}	η / mPa s	φ_V × 10^6/m^3 mol^{-1}
	w_1 = 0.80		
	T = 298.15 K		
0.0024	0.84279	1.0096	177.85
0.0033	0.84300	1.0126	155.41
0.0052	0.84346	1.0251	128.99
0.0071	0.84395	1.0377	110.74
0.0090	0.84448	1.0503	93.93
0.0109	0.84507	1.0639	75.24
	T = 303.15 K		
0.0024	0.83812	0.9693	171.52
0.0033	0.83833	0.9732	150.45
0.0052	0.83879	0.9820	125.32
0.0071	0.83928	0.9926	107.60
0.0090	0.83981	1.0051	91.02
0.0109	0.84041	1.0178	71.09
	T = 313.15 K		
0.0024	0.83005	0.8948	164.63
0.0033	0.83025	0.8987	149.19
0.0052	0.83072	0.9064	120.78
0.0071	0.83121	0.9169	103.47
0.0090	0.83175	0.9266	85.39
0.0109	0.83230	0.9381	72.29
	w_1 = 0.70		
	T = 298.15 K		
0.0023	0.86802	1.1921	175.32
0.0032	0.86822	1.1961	158.86
0.0051	0.86869	1.2081	130.73
0.0069	0.86919	1.2240	107.82
0.0088	0.86971	1.2389	94.96
0.0106	0.87032	1.2597	72.35
	T = 303.15 K		
0.0023	0.86352	1.1470	169.15
0.0032	0.86371	1.1536	158.36
0.0051	0.86419	1.1667	127.30
0.0069	0.86468	1.1799	106.78
0.0088	0.86521	1.1930	92.27
0.0106	0.86582	1.2054	69.69
	T = 313.15 K		
0.0023	0.85574	1.0651	168.44
0.0032	0.85593	1.0708	157.45
0.0051	0.85642	1.0820	123.15
0.0069	0.85691	1.0938	102.96
0.0088	0.85745	1.1066	87.06

TABLE S-II. Continued

m / mol kg^{-1}	ρ×10^{-3} / kg m^{-3}	η / mPa s	φ_V × 10^6/m^3 mol^{-1}
	w_1 = 0.80		
	T = 313.15 K		
0.0106	0.85802	1.1176	69.74
	w_1 = 0.60		
	T = 298.15 K		
0.0022	0.89153	1.4105	172.30
0.0031	0.89172	1.4197	161.56
0.0049	0.89219	1.4321	128.77
0.0067	0.89270	1.4523	106.06
0.0085	0.89321	1.4707	92.97
0.0103	0.89386	1.4912	67.36
	T = 303.15 K		
0.0022	0.88688	1.3734	177.78
0.0031	0.88711	1.3795	148.83
0.0049	0.88756	1.3938	125.41
0.0067	0.88808	1.4091	101.27
0.0085	0.88863	1.4263	82.87
0.0103	0.88918	1.4477	70.89
	T = 313.15 K		
0.0022	0.87925	1.3061	171.46
0.0031	0.87945	1.3121	156.25
0.0049	0.87992	1.3243	124.07
0.0067	0.88045	1.3385	97.58
0.0085	0.88097	1.3537	83.82
0.0103	0.88154	1.3736	68.60

TABLE S-III. Limiting partial molar expansibilities (φ_E^0) for Fe^{III}(salen)Cl in different aqueous methanol solutions at different temperatures; w_1 – mass fraction of methanol

w_1	φ_E^0 ×10^{-3} / m^3 mol^{-1} K^{-1}			S_E×10^{-3} / m^3 kg$^{1/2}$ mol^{-1} K^{-1}			$(\delta\varphi_E^0 / \delta T)_p$ ×10^{-5} m^3 mol^{-1} K^{-2}
	298.15 K	303.15 K	313.15 K	298.15 K	303.15 K	313.15 K	
1.00	–2.158	–2.208	–2.278	13.809	14.152	14.584	–0.785
	(±0.203)	(±0.206)	(±0.214)	(±2.468)	(±2.502)	(±2.600)	(±0.044)
0.90	–1.804	–1.844	–1.898	9.623	9.868	10.130	–0.612
	(±0.085)	(±0.091)	(±0.091)	(±1.060)	(±1.121)	(±1.120)	(±0.035)
0.80	–1.252	–1.277	–1.313	8.491	8.641	8.890	–0.389
	(±0.262)	(±0.265)	(±0.274)	(±1.299)	(±1.33)	(±1.449)	(±0.015)
0.70	–0.550	–0.562	–0.575	1.504	1.558	1.576	–0.160
	(±0.261)	(±0.265)	(±0.272)	(±0.326)	(±0.379)	(±0.347)	(±0.015)
0.60	–0.409	–0.418	–0.427	0.496	0.506	0.518	–0.115
	(±0.319)	(±0.329)	(±0.334)	(±0.146)	(±0.265)	(±0.333)	(±0.011)

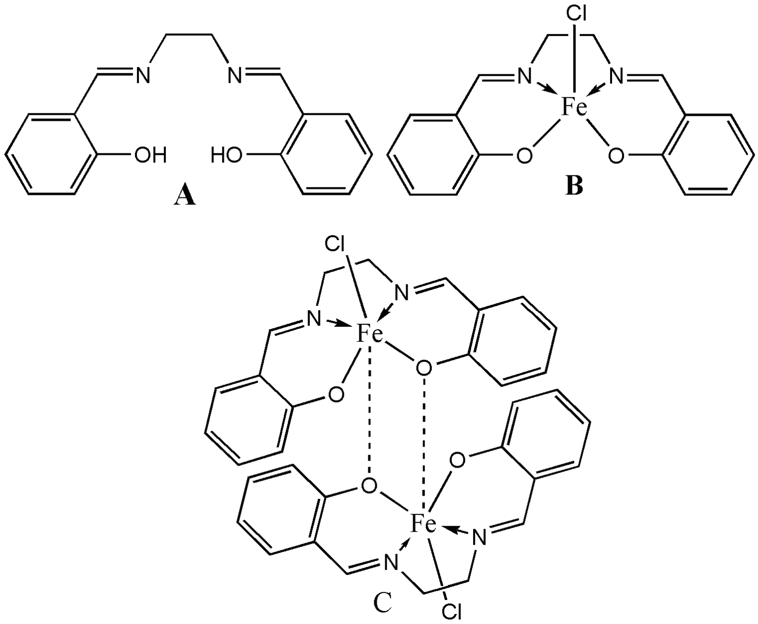

Fig. S-1. Molecular structures of A) salenH_2, B) Fe^{III}(salen)Cl and C) [Fe^{III}(salen)Cl]$_2$.

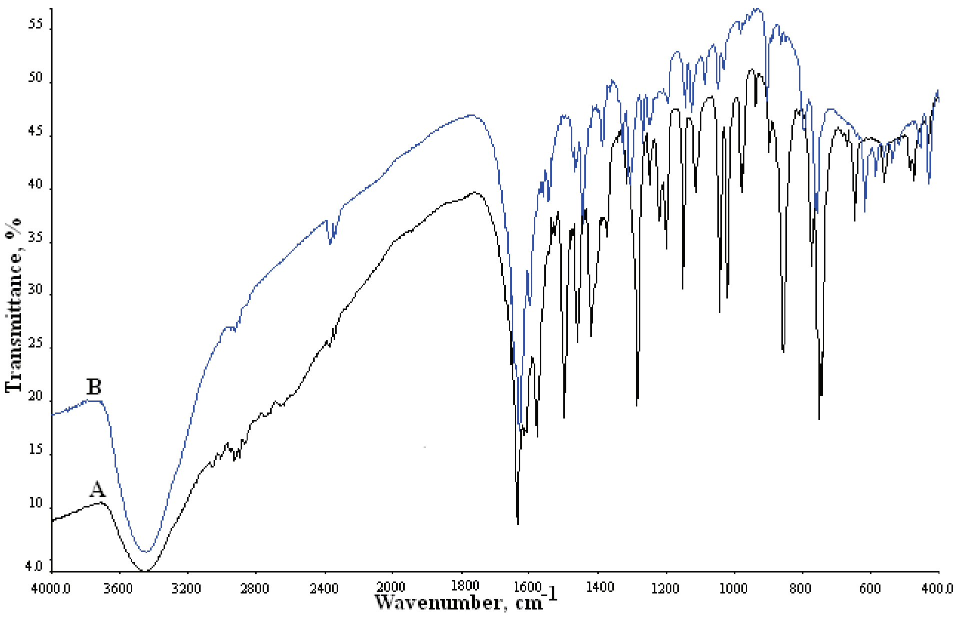

Fig. S-2. IR spectra of A) salenH_2 and B) Fe^{III}(salen)Cl in KBr pellets.

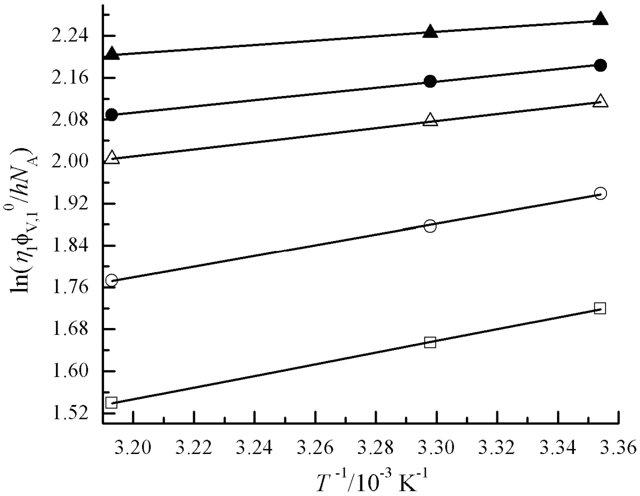

Fig. S-3. Plots of $\ln(\eta_1\varphi^0_{V,1} / hN_A)$ against T^{-1} for Fe^{III}(salen)Cl in aqueous methanol mixtures. Symbols: w_1 = 1.00, □; w_1 = 0.90, ○; w_1 = 0.80, Δ; w_1 = 0.70, ●; w_1 = 0.60, ▲; w_1 is the mass fraction of methanol in the aqueous methanol solutions.

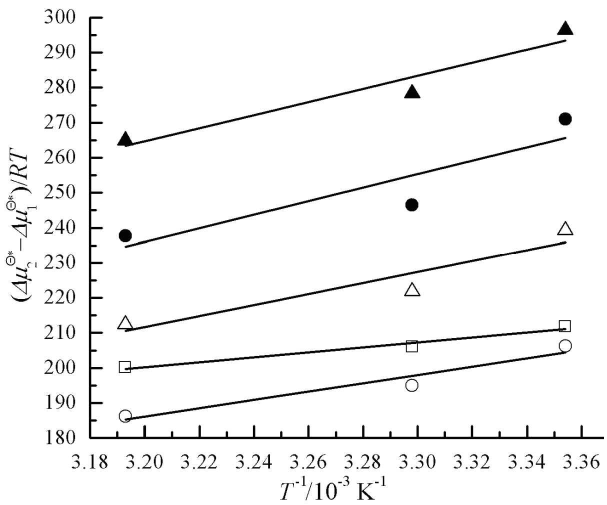

Fig. S-4. Plots of $(\Delta\mu_2^{\ominus*} - \Delta\mu_1^{\ominus*}) / RT$ against T^{-1} for Fe^{III}(salen)Cl in aqueous methanol-water mixtures. Symbols: w_1 = 1.00, □; w_1 = 0.90, ○; w_1 = 0.80, Δ; w_1 = 0.70, ●; w_1 = 0.60, ▲; w_1 is the mass fraction of methanol in the aqueous methanol solutions.

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