

Supplementary Information

Preparation and characterization of iron- β -cyclodextrin inclusion complex: factors influencing the host-guest interaction

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Influence of different factors on IR%, RC% and LC% of iron

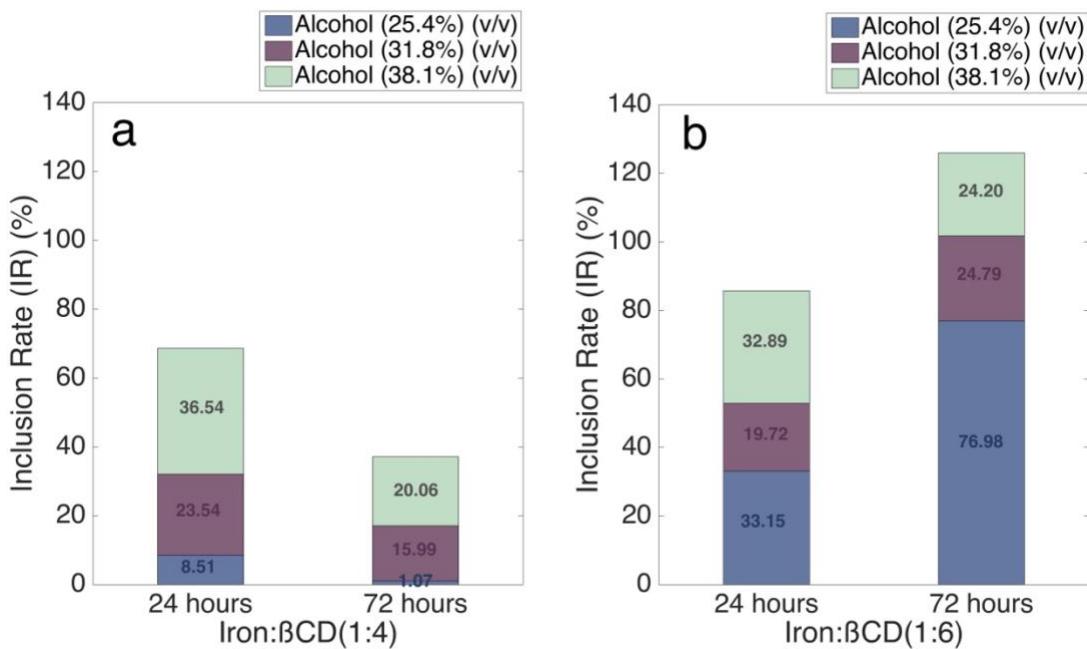


Fig. S1. Influence of stirring time on inclusion rate (IR) (%); a) Iron: β CD (1:4) b) Iron: β CD (1:6)

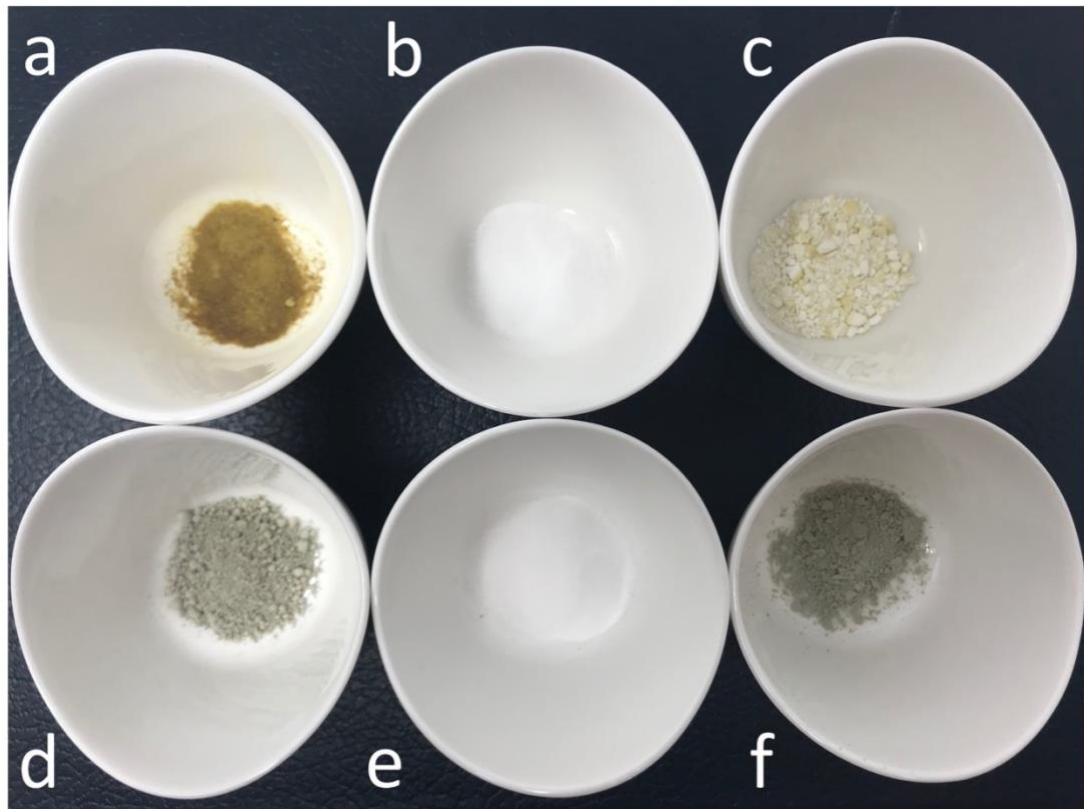


Fig. S2. Images of a) Ferric sodium EDTA (b, e) β CD, c) Ferric sodium EDTA- β CD -IC d) Ferrous ammonium phosphate f) Ferrous ammonium phosphate- β CD -IC

The infrared absorption peaks for iron, β CD, and their inclusion complex

Table S1. The observed infrared absorption peaks and their assigned groups for ferric sodium EDTA (NaFeEDTA), β CD, and NaFeEDTA- β CD ICs.^{1,2}

Ferric sodium EDTA (NaFeEDTA)		β CD		NaFeEDTA- β CD-IC	
IR	Assignment	IR	Assignment	IR	Assignment
3483.12 s	ν_{as} OH	3316.50	ν_{as} OH	3293.94	ν_{as} OH
3371.88 s	ν_{as} OH	2924.13	ν_s CH	2922.28	ν_s CH
3272.8 w		2323.5		2324.3	
2984.5 w	ν (CH ₂)	2190.2		2287.3	
2962.49 w		2168.6		2186.9	
2926.8 w		2113.39		2169.3	
2323.62 w		2083.3		2138	
2162.29 w		1636.85	ν (H-O-H)	2114.90	
2138.51		1412.8	ν (CC)	1982.26	
1982.54		1366.49		1643.11	ν (H-O-H)
1638 vs	ν_{as} (COO ⁻)	1333		1415.61	ν (CC) & δ (CH ₂)
1602.17 sh		1297		1388.24	ν_{as} (COO ⁻)
1463.50 m	δ (CH ₂)	1252.9		1366.13	
1439.84 m		1204.6		1334.03	
1426.63 m		1151.97		1298.76	ν (CC) & δ (CH ₂)
1411.19 m		1100.5	ν (C-O-C)	1252.60	ν (CC)
1378.93 vs	ν_{as} (COO ⁻)	1076.98	ν (CO)	1204.46	ν (CC)
1335.89 m	δ (CH ₂)+ ν (C-CO ₂)	1021.36	ν (CH)	1151.75	
1328.25 m		998.94		1124.08	
1266.27 m	δ (CH ₂)	941.81		1100.93	ν (C-O-C)
1241.01 w		855.05		1076.85	ν (CO)
1217.90 w		756		1020.82	ν (CH)
1174.72 w	ν (CNC)	706.14		998.31	
1103.79 m		605.64		945.95	
1062.22 w	ν_{as} (C ₃ N)	575.32		937.42	
1027.88 w		527.73		861.82	
981.44 w		438.33		753.05	δ (C=O)
964.61 vw		407.36		703.41	
940.84 s				645.63	
926.01 m	ν (CC)			605.65	
877.71 m	ν_{as} Fe-O-Fe			574.96	
838.54 m	ν_s (C ₃ N)			526.95	
751 w	δ (C=O)			475.05	ν (Fe-N)
721.59 s	ρ (CH ₂)			429.05	
669 w	ρ_w (COO ⁻)			402.05	ν (Fe-O)
637.80 m					
598.04 w	π (C=O)				
570.91 m					
538.55 w					
493.01 w					
471.81 m	ν (Fe-N)				
440.84 w					
402.09	ν (Fe-O)				

Table S2. The observed peaks and their assigned groups for ferrous ammonium phosphate, β CD, and ferrous ammonium phosphate- β CD ICs^{3–5}

Ferrous ammonium phosphate (FeNH_4PO_4)		β CD		FeNH_4PO_4 - β CD-IC	
IR	Assignment	IR	Assignment	IR	Assignment
3289.53 s	ν_{as} OH	3316.50	ν_{as} OH	3367.94	ν_{as} OH
2920.49 w	ν (CH_2)	2924.13	ν_{s} CH	2982	ν_{s} CH
2324.55.49 w		2323.5		2889	
		2190.2			
1645.55	ν_{as} (COO^-)	2168.6		1637	$\nu(\text{H-O-H})$
1448		2113.39		1460	
1415.53	ν (NH_2)	2083.3		1432	
		1636.85	$\nu(\text{H-O-H})$	1415	$\nu(\text{NH}_2) + \nu(\text{CC})$
1366.02					
1334.14		1412.8	$\nu(\text{CC})$	1320	
1296.70		1366.49		1248	
1251.66		1333		1206	
1204.11		1297			
1151.64		1252.9			
1100.36		1204.6		1151	
1077.60	ν (PO)	1151.97		1100	$\nu(\text{C-O-C})$
1021.15		1100.5	$\nu(\text{C-O-C})$	1073	$\nu(\text{PO}) + \nu(\text{CO})$
		1076.98	$\nu(\text{CO})$	1023	
946			$\nu(\text{CH})$		
936	ν (P-O-H)	1021.36			
864		998.94		937	$\nu(\text{P-O-H})$
851	ν (Fe)	941.81		755	
753		855.05		729	
705		756		611	
607		706.14		574	$\nu(\text{PO}_4)$
575	ν (PO_4)	605.64		556	
527		575.32		522	
472		527.73		450	
435		438.33		437	
		407.36			

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