Supporting Information

Experimental and computational studies of the influence of cationic Gemini surfactant as corrosion inhibitors for carbon steel in 15% HCl

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Supplementary figures and tables

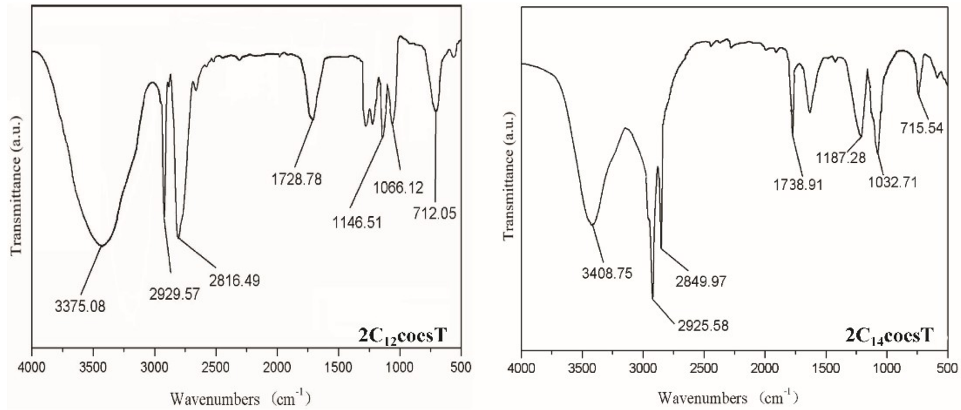

Fig. S1 The FT-IR spectra of $2C_n$coesT (n = 12, 14)

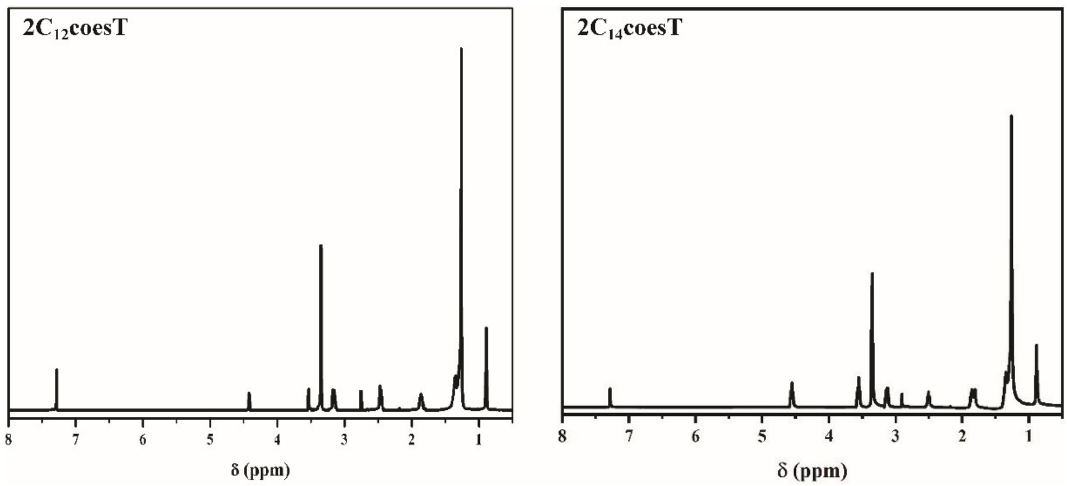

Fig. S2 The ^{1}H NMR spectra of $2C_n$coesT (n = 12, 14)

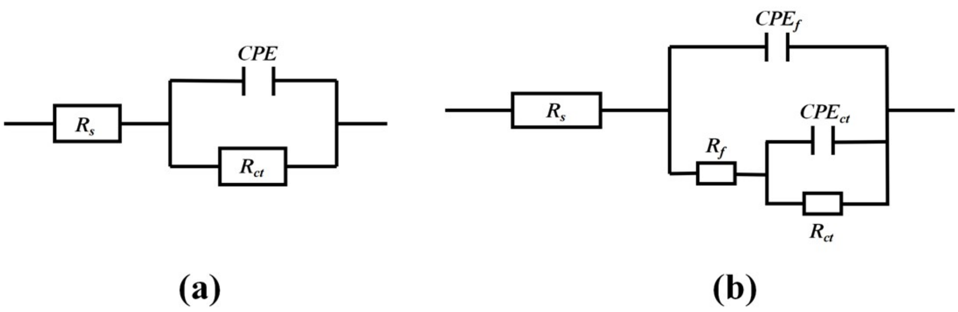

Fig. S3 Equivalent circuit model applied to fit the obtained impedance data.

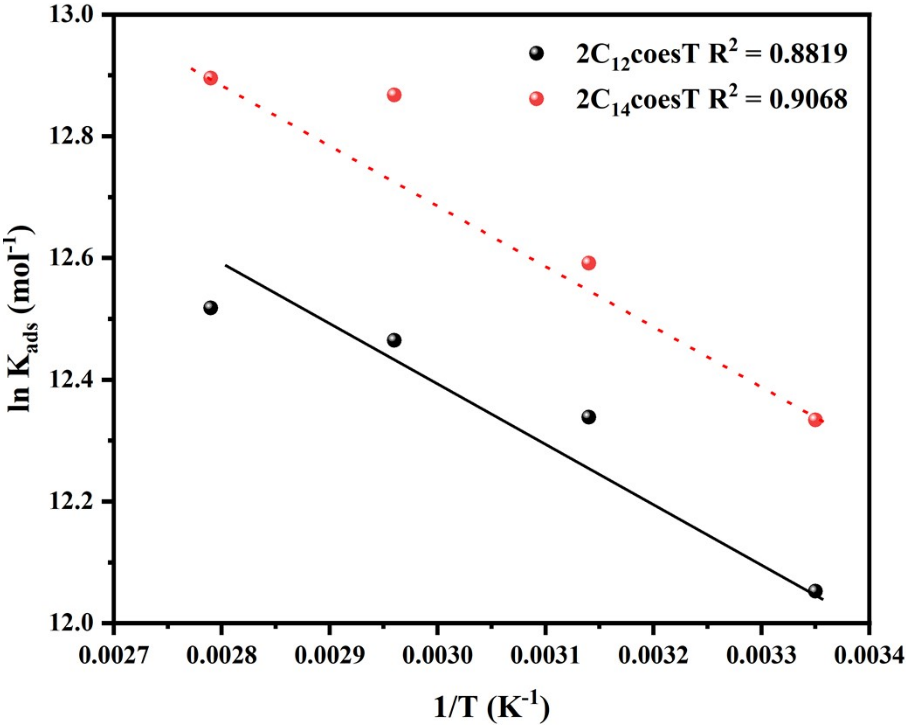

Fig. S4 The relationship between lnK_{ads} and (1/T) for A3 carbon steel in 15% HCl solution with different concentrations of $2C_{12}$coesT and $2C_{14}$coesT.

Table S1 The Fukui indices of surfactant I and II.

Surfactant I				Surfactant II			
Atom	Nucleophilic attack f_k^+	Electrophilic attack f_k^-	Δf_k	Atom	Nucleophilic attack f_k^+	Electrophilic attack f_k^-	Δf_k
O (1)	0.045	0.004	0.041	O (1)	0.047	0.004	0.043
C (2)	0.144	0.007	0.137	C (2)	0.153	0.007	0.146
C (3)	-0.024	-0.007	-0.017	C (3)	-0.023	-0.006	-0.017
C (4)	-0.013	-0.042	0.029	C (4)	-0.013	-0.043	0.03
S (5)	0.034	0.625	-0.591	S (5)	0.034	0.628	-0.594
C (6)	-0.013	-0.042	0.029	C (6)	-0.014	-0.043	0.029
C (7)	-0.024	-0.007	-0.017	C (7)	-0.024	-0.005	-0.019
C (8)	0.163	0.007	0.156	C (8)	0.154	0.007	0.147

O (9)	0.049	0.004	0.045	O (9)	0.047	0.004	0.043
O (10)	0.113	0.01	0.103	O (10)	0.117	0.01	0.107
O (11)	0.122	0.011	0.111	O (11)	0.118	0.01	0.108
C (12)	-0.002	0	-0.002	C (12)	-0.003	0	-0.003
C (13)	-0.015	-0.001	-0.014	C (13)	-0.015	-0.001	-0.014
C (14)	-0.002	0	-0.002	C (14)	-0.003	0	-0.003
C (15)	-0.015	-0.001	-0.014	C (15)	-0.015	-0.001	-0.014
C (16)	-0.002	0	-0.002	C (16)	-0.002	0	-0.002
N (17)	-0.002	0	-0.002	N (17)	-0.002	0	-0.002
C (18)	-0.001	0	-0.001	C (18)	-0.001	0	-0.001
C (19)	-0.002	0	-0.002	C (19)	-0.002	0	-0.002
C (20)	-0.002	0	-0.002	C (20)	-0.002	0	-0.002
N (21)	-0.002	0	-0.002	N (21)	-0.002	0	-0.002
C (22)	-0.002	0	-0.002	C (22)	-0.002	0	-0.002
C (23)	-0.001	0	-0.001	C (23)	-0.001	0	-0.001
C (24)	-0.001	0	-0.001	C (24)	-0.001	0	-0.001
C (25)	0	0	0	C (25)	0	0	0
C (26)	0	0	0	C (26)	0	0	0
C (27)	0	0	0	C (27)	0	0	0
C (28)	0	0	0	C (28)	0	0	0
C (29)	0	0	0	C (29)	0	0	0
C (30)	0	0	0	C (30)	0	0	0
C (31)	0	0	0	C (31)	0	0	0
C (32)	0	0	0	C (32)	0	0	0
C (33)	0	0	0	C (33)	0	0	0
C (34)	0	0	0	C (34)	0	0	0
C (35)	-0.001	0	-0.001	C (35)	-0.001	0	-0.001
C (36)	0	0	0	C (36)	0	0	0
C (37)	0	0	0	C (37)	0	0	0

C (38)	0	0	0	C (38)	0	0	0
C (39)	0	0	0	C (39)	0	0	0
C (40)	0	0	0	C (40)	0	0	0
C (41)	0	0	0	C (41)	0	0	0
C (42)	0	0	0	C (42)	0	0	0
C (43)	0	0	0	C (43)	0	0	0
C (44)	0	0	0	C (44)	0	0	0
C (45)	0	0	0	C (45)	0	0	0
				C (122)	0	0	0
				C (123)	0	0	0
				C (124)	0	0	0
				C (125)	0	0	0