Experimental and Theoretical Investigations of porphyrin Derivatives as Corrosion Inhibitors for Carbon Steel in Acidic Environments

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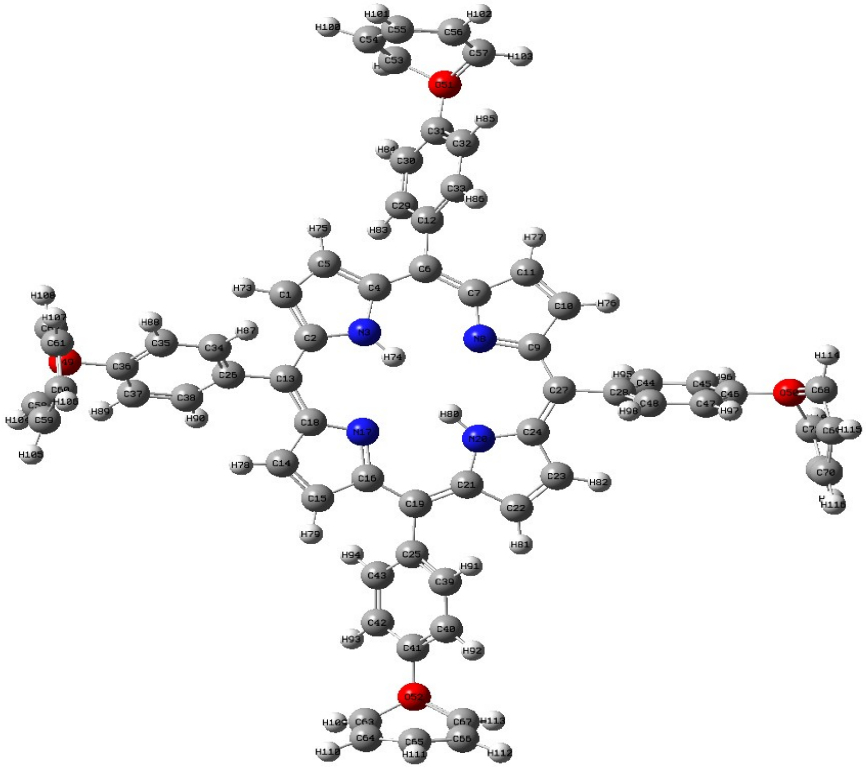

Fig. S1 The optimized geometries of PF-1

Table S1 the calculated Fukui index values of reactive sites on PF-1

Electrophilic Attack (Fukui(-))	Nucleophilic Attack (Fukui(+))	atom
0.012	0.013	C (1)
0.010	0.011	C (2)
0.006	0.007	N (3)
0.009	0.010	C (4)
0.012	0.014	C (5)
0.016	0.018	C (6)
0.010	0.011	C (7)
0.010	0.011	N (8)

0.011	0.011	C (9)
0.011	0.013	C (10)
0.012	0.013	C (11)
-0.004	-0.004	C (12)
0.015	0.016	C (13)
0.012	0.013	C (14)
0.012	0.013	C (15)
0.009	0.010	C (16)
0.010	0.010	N (17)
0.011	0.011	C (18)
0.016	0.018	C (19)
0.006	0.007	N (20)
0.009	0.010	C (21)
0.012	0.013	C (22)
0.012	0.013	C (23)
0.01	0.011	C (24)
-0.003	-0.003	C (25)
-0.004	-0.005	C (26)
0.014	0.016	C (27)
-0.005	-0.006	C (28)
0.004	0.004	C (29)
0.004	0.005	C (30)
0.002	0.002	C (31)
0.003	0.003	C (32)
0.003	0.003	C (33)
0.004	0.004	C (34)
0.003	0.003	C (35)
0.001	0.001	C (36)
0.005	0.005	C (37)
0.004	0.004	C (38)
0.004	0.004	C (39)
0.004	0.004	C (40)
0.001	0.001	C (41)
0.006	0.006	C (42)
0.004	0.005	C (43)
0.004	0.004	C (44)
0.005	0.005	C (45)
0.000	0.000	C (46)
0.003	0.003	C (47)
0.005	0.005	C (48)
0.000	0.000	O (49)
0.000	0.000	O (50)
0.000	0.000	O (51)
0.000	0.000	O (52)
0.016	0.014	C (53)
0.005	0.004	C (54)

0.018	0.016	C (55)
0.003	0.003	C (56)
0.016	0.014	C (57)
0.019	0.017	C (58)
0.005	0.005	C (59)
0.020	0.018	C (60)
0.003	0.003	C (61)
0.018	0.017	C (62)
0.023	0.022	C (63)
0.006	0.005	C (64)
0.024	0.023	C (65)
0.003	0.003	C (66)
0.023	0.021	C (67)
0.022	0.020	C (68)
0.003	0.003	C (69)
0.023	0.021	C (70)
0.005	0.005	C (71)
0.022	0.020	C (72)

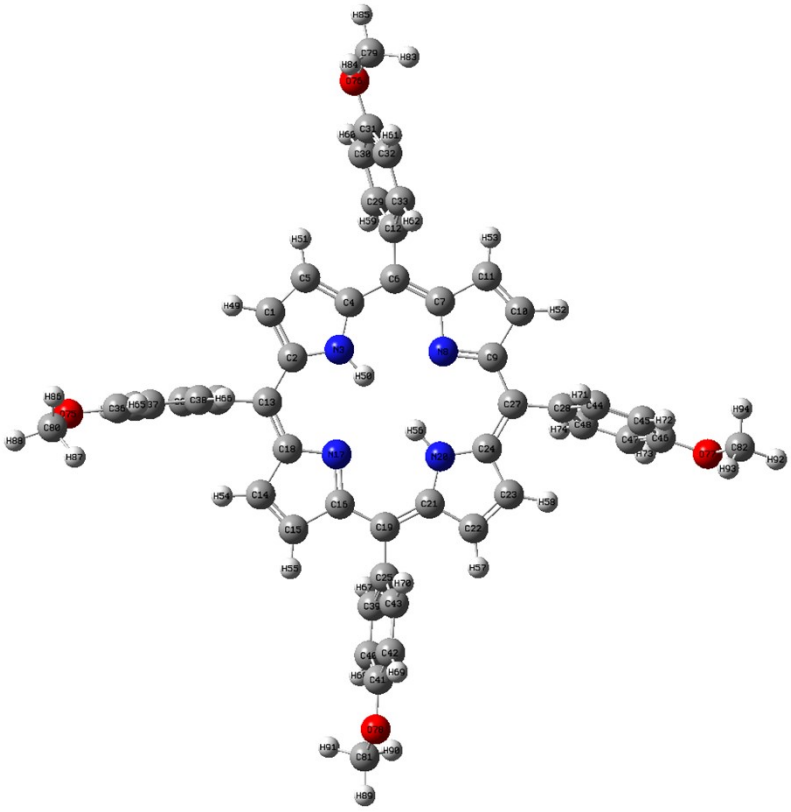

Fig. S2 The optimized geometries of PF-2

Table S2 the calculated Fukui index values of reactive sites on PF-2

Electrophilic Attack (Fukui(-))	Nucleophilic Attack (Fukui(+))	atom
0.016	0.025	C (1)
0.013	0.02	C (2)
0.015	0.014	N (3)
0.013	0.02	C (4)
0.016	0.025	C (5)
0.038	0.036	C (6)
0.011	0.019	C (7)
0.026	0.021	N (8)
0.012	0.020	C (9)
0.012	0.024	C (10)
0.012	0.024	C (11)
-0.003	-0.008	C (12)
0.037	0.034	C (13)
0.012	0.024	C (14)
0.013	0.025	C (15)
0.012	0.02	C (16)
0.027	0.021	N (17)
0.012	0.02	C (18)
0.038	0.034	C (19)
0.015	0.014	N (20)
0.013	0.02	C (21)
0.016	0.026	C (22)
0.016	0.025	C (23)
0.013	0.02	C (24)
-0.005	-0.01	C (25)
-0.004	-0.009	C (26)
0.037	0.034	C (27)
-0.004	-0.009	C (28)
0.007	0.004	C (29)
0.01	0.007	C (30)
0.011	0.008	C (31)
0.01	0.006	C (32)
0.009	0.005	C (33)
0.007	0.004	C (34)
0.01	0.007	C (35)
0.011	0.008	C (36)
0.009	0.006	C (37)
0.008	0.005	C (38)
0.008	0.004	C (39)
0.009	0.006	C (40)
0.01	0.007	C (41)
0.009	0.006	C (42)
0.006	0.003	C (43)
0.008	0.005	C (44)

0.009	0.006	C (45)
0.011	0.008	C (46)
0.01	0.007	C (47)
0.007	0.004	C (48)
0.012	0.006	O (75)
0.012	0.006	O (76)
0.011	0.005	O (77)
0.011	0.005	O (78)
-0.003	-0.002	C (79)
-0.003	-0.002	C (80)
-0.003	-0.002	C (81)
-0.003	-0.002	C (82)