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Supplementary Material

Experimental and computational study of a multi-active-site Schiff base as corrosion inhibitor of mild steel in 1 M HCl

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Table S1. Comparison of the corrosion inhibition efficiencies by weight loss test of some Schiff bases reported in 1.0 M HCl on mild steel.

Schiff base	Type	Mol. weight ($g\ mol^{-1}$)	C_{inh} ($mmol\ L^{-1}$)	T (K)	η_w (%)	Ref.
4-(4-((pyridin-2-yl)methyleneamino)-phenoxy)-N-((pyridin-2-yl)methylene)-benzenamine [PMB]	double	378.37	5.0	298	88	[15]
4-(4-(4-((pyridin-2-yl)methyleneamino)-phenoxy)phenoxy)-N-((pyridin-2-yl)-methylene)benzenamine [PPMB]	double	470.45	5.0	298	92	[15]
N,N'-dibenzo[*b*,*d*]thiene-2,8-diylbis(1-(thiophen-2-yl)methanimine) [SB]	double	402.50	1.0	298	92.95	[24]
(1E,1'E)-N,N'-(1,4-phenylene)bis(1-(pyridin-2-yl)methanimine) [PBPE2]	double	286.27	2.8	303	91.88	[28]
(1E,1'E)-N,N'-(1,4-phenylene)bis(1-(pyridin-3-yl)methanimine) [PBPE3]	double	286.27	2.8	303	92.18	[28]
2-((4-(dimethylamino)benzylidene)-amino)benzenethiol [DBB]	single	256.32	2.0	298	78.6 (η_{EIS})	[37]
3-[(3-Hydroxy-4-methoxy-benzylidene)-amino]benzoic acid [HMAMB]	single	271.23	1.0	303	87.53 (η_{EIS})	[38]
3-[(2-Hydroxy-naphthalen-1-ylmethylene)-amino]benzoic acid [HNCAMB]	single	291.13	1.0	303	89.13 (η_{EIS})	[38]
N,N'-(1,4-phenylene)bis(1,1-di(pyridin-2-yl)methanimine) [PBDPM]	double	440.17	1.8	303	93.76	This work

Table S2. The bond length and bond angle parameters of PBDPM.

PBDPM	Bond angle (°)	PBDPM	Bond length (Å)	PBDPM	Bond angle (°)	PBDPM	Bond length (Å)
C_1–C_2–C_3	120.798	C_1–C_2	1.406	N_{13}–C_{14}–C_{15}	123.658	C_{14}–C_{15}	1.399
C_2–C_3–C_4	120.616	C_2–C_3	1.393	C_{14}–C_{15}–C_{16}	118.043	C_{15}–C_{16}	1.394
C_3–C_4–C_5	118.458	C_3–C_4	1.407	C_{15}–C_{16}–C_{17}	118.685	C_{16}–C_{17}	1.395
C_4–C_5–C_6	120.800	C_4–C_5	1.409	C_{16}–C_{17}–C_8	118.968	C_{17}–C_9	1.405
C_5–C_6–C_1	120.671	C_5–C_6	1.389	N_7–C_8–C_{44}	117.149	C_8–C_{44}	1.509
C_6–C_1–C_2	118.511	C_6–C_1	1.408	C_8–C_{44}–C_{45}	120.877	C_{44}–C_{45}	1.404
C_2–C_1–N_7	122.590	C_1–N_7	1.399	C_{44}–C_{45}–N_{47}	118.748	C_{45}–C_{47}	1.395
C_1–N_7–C_8	124.982	N_7–C_8	1.273	C_{45}–C_{47}–C_{49}	118.707	C_{47}–C_{49}	1.395
C_8–C_9–N_{13}	117.936	C_8–C_9	1.502	C_{47}–C_{49}–C_{46}	118.188	C_{49}–C_{46}	1.398
C_9–C_{16}–C_{17}	117.266	C_9–N_{13}	1.340	C_{49}–C_{46}–N_{54}	123.443	C_{46}–N_{54}	1.331
C_{17}–N_{13}–C_{14}	118.521	N_{13}–C_{14}	1.329	C_{46}–N_{54}–C_{44}	118.498	N_{54}–C_{44}	1.338

Table S3. Fukui index of PBDPM.

PBDPM	f_k^+	f_k^-	PBDPM	f_k^+	f_k^-
C_1	–0.054	–0.029	C_{18}	–0.019	0.003
C_2	–0.010	–0.035	C_{19}	–0.013	–0.004
C_3	–0.009	–0.038	C_{20}	–0.026	–0.015
C_4	–0.002	–0.006	C_{21}	0.003	–0.003
C_5	–0.002	–0.021	N_{22}	–0.025	0.003
C_6	–0.004	–0.048	C_{35}	–0.028	–0.012
N_7	–0.078	–0.030	C_{36}	0.002	0.032
C_8	–0.020	–0.036	C_{37}	–0.005	–0.003
C_9	0.041	0.010	C_{38}	–0.011	–0.009
N_{10}	–0.071	–0.060	C_{40}	–0.019	–0.014
C_{11}	–0.036	–0.039	C_{44}	–0.013	–0.079
C_{12}	0.055	–0.052	C_{45}	0.020	0.037
N_{13}	–0.027	0.001	C_{46}	–0.005	0.003
C_{14}	0.004	–0.001	C_{47}	–0.006	–0.016
C_{15}	–0.024	–0.011	C_{49}	–0.019	–0.017
C_{16}	–0.013	–0.005	N_{53}	–0.005	–0.025
C_{17}	–0.001	0.002	N_{54}	–0.053	0.030

References

[15] M Murmu, SK Saha, NC Murmu, P Banerjee, Effect of stereochemical conformation into the corrosion inhibitive behaviour of double azomethine based Schiff bases on mild steel surface in 1 mol L^{-1} HCl medium: an experimental, density functional theory and molecular dynamics simulation study. *Corros Sci* 2019, 146, 134-151.

[24] N Karki, S Neupane, DK Gupta, AK Das, S Singh, GM Koju, Y Chaudhary, AP Yadav, Berberine isolated from *Mahonia nepalensis* as an eco-friendly and thermally stable corrosion inhibitor for mild steel in acid medium. *Arab J Chem* 2021, 14, 103423.

[28] LX Li, B Xie, C Lai, JS Feng, XQ Liu, L Chen, YG Yang, RW Ji, JY He, W Li, ML Liu, Adsorption and corrosion inhibition performance of two planar rigid pyridinecarboxaldehyde-based double Schiff bases for mild steel in HCl solution: experimental and computational investigations. *J Mol Liq* 2022, 355, 118926.

[37] W Guo, M Talha, Y Lin, X Kong, Schiff's base with center of symmetry as an effective corrosion inhibitor for mild steel in acid medium: electrochemical & simulation studies. *Colloid Surf A – Physicochem Eng Asp* 2021, 615, 126234.

[38] KT Loganathan, ST Venkatesan, S Nagarajan, R Natarajan, Corrosion inhibitive evaluation and DFT studies of 2-(Furan-2-yl)-4,5-diphenyl-1H-imidazole on mild steel at 1.0 M HCl. *J Indian Chem Soc* 2021, 98, 100121.