# Supplementary Data

## Anticorrosion Potential of 4-Amino-3-methyl-1,2,4-triazole-5-thione Derivatives (SAMTT and DBAMTT) on Mild Steel in Hydrochloric Acid Solution

**Moorthy Saravana Kumar, Saravana Loganathan Ashok Kumar and Anandaram Sreekanth***

Department of Chemistry, Centre of Excellence in Corrosion and Surface Engineering, National Institute of Technology-Tiruchirappalli, Tiruchirappalli 620015, Tamilnadu, India.

* Corresponding Author
Dr. A. Sreekanth, Assistant Professor, Department of Chemistry, Centre of Excellence in Corrosion and Surface Engineering, National Institute of Technology-Tiruchirappalli, Tiruchirappalli-620015, Tamilnadu, India
E-mail: sreekanth@nitt.edu
Tel: +91 431 2503642
Fax: +91 431 2500133

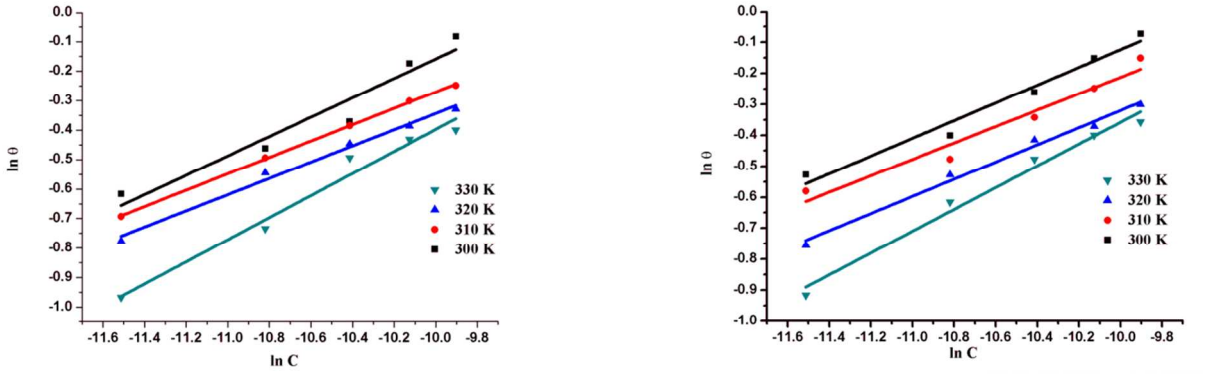


**Figure S1**. Freundlich adsorption plots on mild steel in 1 M HCl at different temperature, EIS (300 K) and Tafel Polarization (300 K). (A) Different temperature of SAMTT and (B) Different temperature of DBAMTT.

**Table S1**. Inhibition efficiency obtained by weight loss of mild steel in 1 M HCl containing various concentrations of AMTT, SAMTT & DBAMTT at 300 K.

| **AMTT** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Inhibitor conc. ($10^{-4}$mol/L) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Average | IE (%) | CR (mg/ $cm^{-2}h^{-1}$) | $\theta$ | $\sigma^{b}$ | Error of Margin |
| Blank | 236.10 | 236.10 | 236.10 | 236.1 | | 1.64 | | 0.00 | |
| 1.0 | 118.24 | 118.22 | 118.10 | 118.2 | 50 | 0.82 | 0.50 | 0.08 | 0.26 |
| 2.0 | 96.23 | 96.28 | 96.17 | 96.2 | 59 | 0.67 | 0.59 | 0.06 | 0.19 |
| 3.0 | 84.52 | 84.49 | 84.50 | 84.5 | 64 | 0.59 | 0.64 | 0.02 | 0.05 |
| 4.0 | 74.33 | 74.28 | 74.37 | 74.3 | 69 | 0.52 | 0.69 | 0.05 | 0.16 |
| 5.0 | 67.28 | 67.27 | 67.39 | 67.3 | 71 | 0.47 | 0.71 | 0.07 | 0.23 |
| 6.0 | 66.99 | 66.97 | 66.94 | 67.0 | 72 | 0.47 | 0.72 | 0.03 | 0.09 |
| 7.0 | 64.76 | 64.74 | 64.72 | 64.7 | 73 | 0.45 | 0.73 | 0.02 | 0.07 |
| **SAMTT** | | | | | | | | | |
| 1.0 | 108.23 | 108.13 | 108.10 | 108.2 | 54 | 0.75 | 0.54 | 0.07 | 0.24 |
| 2.0 | 88.21 | 88.30 | 88.30 | 88.3 | 63 | 0.61 | 0.63 | 0.05 | 0.18 |
| 3.0 | 72.40 | 72.49 | 72.53 | 72.5 | 69 | 0.50 | 0.69 | 0.07 | 0.23 |
| 4.0 | 37.50 | 37.49 | 37.54 | 37.5 | 84 | 0.26 | 0.84 | 0.03 | 0.09 |
| 5.0 | 19.19 | 19.25 | 19.36 | 19.3 | 92 | 0.13 | 0.92 | 0.09 | 0.30 |
| 6.0 | 18.89 | 18.98 | 18.96 | 18.9 | 92 | 0.13 | 0.92 | 0.05 | 0.16 |
| 7.0 | 17.59 | 17.40 | 17.45 | 17.5 | 93 | 0.12 | 0.93 | 0.10 | 0.34 |
| **DBAMTT** | | | | | | | | | |
| 1.0 | 97.24 | 97.19 | 97.22 | 97.2 | 59 | 0.68 | 0.59 | 0.03 | 0.09 |
| 2.0 | 78.72 | 78.81 | 78.71 | 78.7 | 67 | 0.55 | 0.67 | 0.06 | 0.19 |
| 3.0 | 54.51 | 54.36 | 54.51 | 54.5 | 77 | 0.38 | 0.77 | 0.09 | 0.30 |
| 4.0 | 32.30 | 32.29 | 32.35 | 32.3 | 86 | 0.22 | 0.86 | 0.03 | 0.11 |
| 5.0 | 17.35 | 17.46 | 17.48 | 17.4 | 93 | 0.12 | 0.93 | 0.07 | 0.24 |
| 6.0 | 16.14 | 16.26 | 16.22 | 16.2 | 93 | 0.11 | 0.93 | 0.06 | 0.21 |
| 7.0 | 15.25 | 15.27 | 15.28 | 15.3 | 94 | 0.11 | 0.94 | 0.02 | 0.05 |

[a] Weight loss shown is the mean of triplicate measurements

[b] Standard deviation ($\sigma$) listed is calculated for different weight loss measurements

**Table S2.** Inhibition efficiency obtained by weight loss of mild steel in 1 M HCl containing various concentrations of AMTT, SAMTT & DBAMTT at 310 K

| **AMTT** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Inhibitor conc. ($10^{-4}$mol/ L) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Average | IE (%) | CR (mg/ $cm^{-2}$ $h^{-1}$) | $\theta$ | $\sigma^{b}$ | Error of Margin |
| Blank | 306.1 | 306.1 | 306.1 | 306.1 | | 2.13 | | 0.02 | 0.05 |
| 1.0 | 231.2 | 231.2 | 231.3 | 231.2 | 24 | 1.61 | 0.24 | 0.06 | 0.20 |
| 2.0 | 188.3 | 188.4 | 188.4 | 188.4 | 38 | 1.31 | 0.38 | 0.05 | 0.18 |
| 3.0 | 155.7 | 155.6 | 155.6 | 155.6 | 49 | 1.08 | 0.49 | 0.07 | 0.25 |
| 4.0 | 133.5 | 133.6 | 133.7 | 133.6 | 56 | 0.93 | 0.56 | 0.08 | 0.26 |
| 5.0 | 119.6 | 119.6 | 119.5 | 119.6 | 61 | 0.83 | 0.61 | 0.09 | 0.30 |
| **SAMTT** | | | | | | | | | |
| 1.0 | 153.01 | 153.03 | 153.14 | 153.1 | 50 | 1.06 | 0.50 | 0.07 | 0.24 |
| 2.0 | 120.50 | 120.46 | 120.52 | 120.5 | 61 | 0.84 | 0.61 | 0.03 | 0.11 |
| 3.0 | 97.40 | 97.45 | 97.35 | 97.4 | 68 | 0.68 | 0.68 | 0.05 | 0.17 |
| 4.0 | 79.35 | 79.39 | 79.51 | 79.4 | 74 | 0.55 | 0.74 | 0.08 | 0.29 |
| 5.0 | 66.89 | 66.89 | 66.99 | 66.9 | 78 | 0.47 | 0.78 | 0.06 | 0.20 |
| **DBAMTT** | | | | | | | | | |
| 1.0 | 136.03 | 135.89 | 136.00 | 102.0 | 56 | 0.94 | 0.56 | 0.07 | 0.26 |
| 2.0 | 114.76 | 114.77 | 114.81 | 136.0 | 62 | 0.80 | 0.62 | 0.03 | 0.09 |
| 3.0 | 87.51 | 87.56 | 87.45 | 114.8 | 71 | 0.61 | 0.71 | 0.06 | 0.19 |
| 4.0 | 66.01 | 66.04 | 66.02 | 87.5 | 78 | 0.46 | 0.78 | 0.02 | 0.05 |
| 5.0 | 42.25 | 42.19 | 42.22 | 66.0 | 86 | 0.29 | 0.86 | 0.03 | 0.10 |

[a] Weight loss shown is the mean of triplicate measurements

[b]Standard deviation ($\sigma$) listed is calculated for different weight loss measurements

**Table S3.** Inhibition efficiency obtained by weight loss of mild steel in 1 M HCl containing various concentrations of AMTT, SAMTT & DBAMTT at 320 K

| **AMTT** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Inhibitor conc. ($10^{-4}$mol/L) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Average | IE (%) | CR (mg/ $cm^{-2}$ $h^{-1}$) | $\theta$ | $\sigma^{b}$ | Error of Margin |
| Blank | 507.3 | 507.3 | 507.3 | 507.3 | | 3.52 | | 0.00 | 0.00 |
| 1.0 | 407.7 | 407.8 | 407.8 | 407.8 | 20 | 2.83 | 0.20 | 0.08 | 0.26 |
| 2.0 | 343.6 | 343.7 | 343.7 | 343.6 | 32 | 2.38 | 0.32 | 0.03 | 0.10 |
| 3.0 | 298.6 | 298.7 | 298.6 | 298.6 | 41 | 2.07 | 0.41 | 0.06 | 0.20 |
| 4.0 | 256.9 | 256.8 | 256.8 | 256.8 | 49 | 1.78 | 0.49 | 0.07 | 0.24 |
| 5.0 | 228.5 | 228.6 | 228.6 | 228.5 | 55 | 1.59 | 0.55 | 0.03 | 0.12 |
| **SAMTT** | | | | | | | | | |
| 1.0 | 276.28 | 276.24 | 276.16 | 276.2 | 46 | 1.92 | 0.50 | 0.06 | 0.21 |
| 2.0 | 213.26 | 213.39 | 213.31 | 213.3 | 58 | 1.48 | 0.61 | 0.07 | 0.23 |
| 3.0 | 182.37 | 182.33 | 182.28 | 182.3 | 64 | 1.27 | 0.68 | 0.05 | 0.16 |
| 4.0 | 164.24 | 164.21 | 164.28 | 164.2 | 68 | 1.14 | 0.74 | 0.04 | 0.12 |
| 5.0 | 140.27 | 140.19 | 140.23 | 140.2 | 72 | 0.97 | 0.78 | 0.04 | 0.14 |
| **DBAMTT** | | | | | | | | | |
| 1.0 | 267.68 | 267.72 | 267.73 | 267.7 | 47 | 1.86 | 0.47 | 0.03 | 0.09 |
| 2.0 | 207.35 | 207.45 | 207.48 | 207.4 | 59 | 1.44 | 0.59 | 0.07 | 0.24 |
| 3.0 | 170.42 | 170.48 | 170.40 | 170.4 | 66 | 1.18 | 0.66 | 0.04 | 0.14 |
| 4.0 | 155.38 | 155.42 | 155.40 | 155.4 | 69 | 1.08 | 0.68 | 0.02 | 0.07 |
| 5.0 | 132.64 | 132.74 | 132.61 | 132.7 | 74 | 0.92 | 0.74 | 0.07 | 0.24 |

[a] Weight loss shown is the mean of triplicate measurements

[b] Standard deviation ($\sigma$) listed is calculated for different weight loss measurements

**Table S4.** Inhibition efficiency obtained by weight loss of mild steel in 1 M HCl containing various concentrations of AMTT, SAMTT & DBAMTT at 330 K

| **AMTT** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Inhibitor conc. ($10^{-4}$mol/L) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Average | IE (%) | CR (mg/ $cm^{-2}$ $h^{-1}$) | $\theta$ | $\sigma^{b}$ | Error of Margin |
| Blank | 604.2 | 604.2 | 604.2 | 604.2 | | 4.20 | | 0.00 | 0.00 |
| 1.0 | 494.5 | 494.5 | 494.4 | 494.5 | 18 | 3.43 | 0.18 | 0.09 | 0.30 |
| 2.0 | 418.3 | 418.4 | 418.3 | 418.3 | 31 | 2.90 | 0.31 | 0.06 | 0.21 |
| 3.0 | 368.7 | 368.7 | 368.8 | 368.7 | 39 | 2.56 | 0.39 | 0.06 | 0.20 |
| 4.0 | 316.6 | 316.5 | 316.5 | 316.5 | 48 | 2.20 | 0.48 | 0.06 | 0.21 |
| 5.0 | 289.6 | 289.6 | 289.7 | 289.6 | 52 | 2.01 | 0.52 | 0.08 | 0.26 |
| **SAMTT** | | | | | | | | | |
| 1.0 | 376.25 | 376.25 | 376.12 | 376.2 | 38 | 2.61 | 0.38 | 0.08 | 0.26 |
| 2.0 | 315.55 | 315.69 | 315.6 | 315.6 | 48 | 2.19 | 0.48 | 0.07 | 0.25 |
| 3.0 | 234.43 | 234.44 | 234.5 | 234.5 | 61 | 1.63 | 0.61 | 0.04 | 0.13 |
| 4.0 | 212.25 | 212.29 | 212.3 | 212.3 | 65 | 1.47 | 0.65 | 0.03 | 0.09 |
| 5.0 | 196.69 | 196.68 | 196.7 | 196.7 | 67 | 1.37 | 0.67 | 0.01 | 0.03 |
| **DBAMTT** | | | | | | | | | |
| 1.0 | 361.75 | 361.85 | 361.75 | 361.8 | 40 | 2.51 | 0.40 | 0.06 | 0.20 |
| 2.0 | 277.63 | 277.70 | 277.60 | 277.6 | 54 | 1.93 | 0.54 | 0.05 | 0.18 |
| 3.0 | 229.69 | 229.68 | 229.70 | 229.7 | 62 | 1.60 | 0.62 | 0.01 | 0.03 |
| 4.0 | 201.38 | 201.42 | 201.44 | 201.4 | 67 | 1.40 | 0.67 | 0.03 | 0.11 |
| 5.0 | 178.72 | 178.65 | 178.70 | 178.7 | 70 | 1.24 | 0.70 | 0.04 | 0.12 |

[a] Weight loss shown is the mean of triplicate measurements

[b]Standard deviation (σ) listed is calculated for different weight loss measurements

**Table S5.** Inhibition efficiency obtained by weight loss of mild steel in 1 M HCl containing various concentrations of Salicylaldehyde & 2,4-dihydroxybenzaldehyde at 300 K

| **Salicylaldehyde** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Inhibitor conc. ($10^{-4}$mol /L) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Weight loss[a] (mg $cm^{-2}$) | Average | IE (%) | CR (mg/ $cm^{-2}$ $h^{-1}$) | $\theta$ | $\sigma^{b}$ | Error of Margin |
| Blank | 236.1 | 236.1 | 236.1 | 236.1 | | 1.64 | | 0.00 | 0.00 |
| 1.0 | 218.27 | 218.21 | 218.20 | 218.2 | 8 | 1.52 | 0.08 | 0.04 | 0.13 |
| 2.0 | 209.28 | 209.22 | 209.20 | 209.2 | 11 | 1.45 | 0.11 | 0.04 | 0.14 |
| 3.0 | 202.58 | 202.52 | 202.50 | 202.5 | 14 | 1.41 | 0.14 | 0.04 | 0.14 |
| 4.0 | 198.35 | 198.36 | 198.30 | 198.3 | 16 | 1.38 | 0.16 | 0.03 | 0.11 |
| 5.0 | 194.32 | 194.37 | 194.31 | 194.3 | 18 | 1.35 | 0.18 | 0.03 | 0.11 |
| 6.0 | 189.93 | 189.93 | 189.99 | 190.0 | 20 | 1.32 | 0.20 | 0.03 | 0.12 |
| 7.0 | 185.75 | 185.76 | 185.78 | 185.8 | 21 | 1.29 | 0.21 | 0.02 | 0.05 |
| **2,4-dihydroxybenzaldehyde** | | | | | | | | | |
| 1.0 | 202.21 | 202.25 | 202.2 | 202.2 | 14 | 1.40 | 0.14 | 0.03 | 0.09 |
| 2.0 | 198.43 | 198.45 | 198.46 | 198.4 | 16 | 1.38 | 0.16 | 0.02 | 0.05 |
| 3.0 | 186.62 | 186.63 | 186.65 | 186.6 | 21 | 1.30 | 0.21 | 0.02 | 0.05 |
| 4.0 | 183.64 | 183.7 | 183.6 | 183.6 | 22 | 1.28 | 0.22 | 0.05 | 0.17 |
| 5.0 | 178.67 | 178.72 | 178.71 | 178.6 | 24 | 1.24 | 0.24 | 0.03 | 0.09 |
| 6.0 | 172.90 | 172.93 | 172.99 | 172.99 | 27 | 1.20 | 0.27 | 0.05 | 0.16 |
| 7.0 | 169.73 | 169.75 | 169.77 | 169.76 | 28 | 1.18 | 0.28 | 0.02 | 0.07 |

[a] Weight loss shown is the mean of triplicate measurements

[b] Standard deviation ($\sigma$) listed is calculated for different weight loss measurements

**Table S6.** Estimation of the equilibrium adsorption constant ($K_{ads}$) and the free energy of adsorption ($\Delta G^0_{ads}$) of SAMTT and DBAMTT on mild steel surface immersed in 1 M HCl solution using Freundlich isotherm.

| Temperature (K) | Freundlich Isotherm Model | | | |
|---|---|---|---|---|
| | Corelation coefficient ($r^2$) | Adsorption Constant $K_{ads}$ ($M^{-1}$) | n | $\Delta G^0_{ads}$ kJ $mol^{-1}$ |
| **SAMTT** | | | | |
| 300 | 0.92 | 22.84 | 0.328 | 17.82 |
| 310 | 0.99 | 12.28 | 0.277 | 16.81 |
| 320 | 0.98 | 11.14 | 0.275 | 17.10 |
| 330 | 0.96 | 28.42 | 0.374 | 20.20 |
| **DBAMTT** | | | | |
| 300 | 0.96 | 15.44 | 0.286 | 16.84 |
| 310 | 0.94 | 11.45 | 0.265 | 16.63 |
| 320 | 0.98 | 11.65 | 0.277 | 17.21 |
| 330 | 0.97 | 23.59 | 0.351 | 19.70 |