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# Alkylphenyl-substituted imidazolines as corrosion inhibitors: experimental and DFT study

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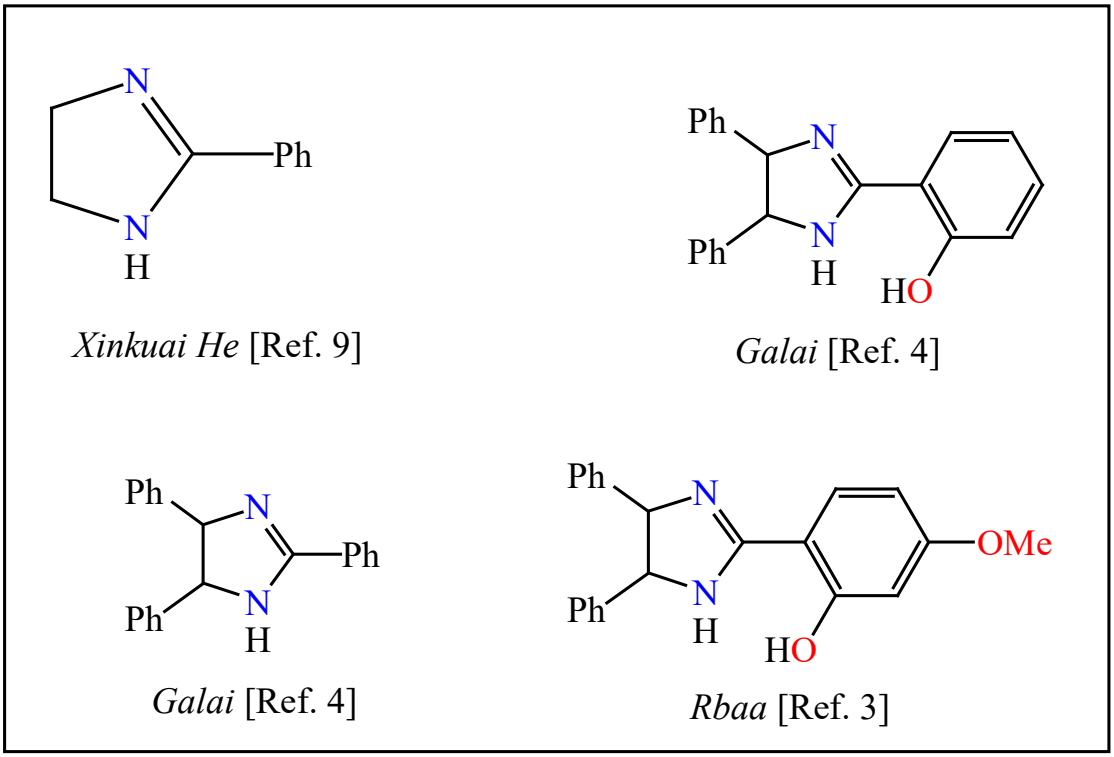



**Figure S1** Corrosion inhibitors based on imidazoline core.

## General information

$^{1}H$ and $^{13}C$ NMR spectra were recorded at 298 K on Bruker Avance 300 spectrometer with operating frequencies of 400 and 100 MHz, respectively, and calibrated using residual $CHCl_3$ ($\delta_H$ = 7.26 ppm) and $CDCl_3$ ($\delta_C$ = 77.16 ppm). NMR data were presented as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, m = multiplet), coupling constant (J) in Hertz (Hz), integration.

Determination of steel corrosion rate by measuring the mass loss of metal samples was carried out using scales GR-202 (AND Company, Japan).

Temperature maintenance of vessels with acid solutions during corrosion tests was carried out using a circulating thermostat LOIP LT-411a (CJSC "Laboratory Equipment and Instrumentation" (abbreviated LOIP), Russia).

The calculations were performed on a laptop ASUS TUF Gaming F17 FX706 (Intel Core i5-11400H, 16GB RAM, 512+1024 GB SSD, 4GB GeForce RTX 3050 Ti Mobile). For DFT calculations Schrödinger 2023.1 program (https://www.schrodinger.com/) was used (module Jaguar, B3LYP, QM Basic 6-31g**, solvent model PBF, water). For MD calculations Forcite module (NVT ensemble, 95°C, Andersen thermostat, timestep 1 fs, time 100 ps, COMPASSIII forcefield) of BIOVIA Materials Studio 2023 (https://www.3ds.com/products/biovia/materials-studio) was used.

## Gravimetric analysis data

**Table S1.** Influence of imidazoline derivatives **4-6**, urotropine and their mixtures on the corrosion rate of 08PS steel in 2 M HCl ($k$/g m$^{-2}$ h$^{-1}$), the corrosion inhibition factors ($\gamma$), and the degree of protection (Z/%).

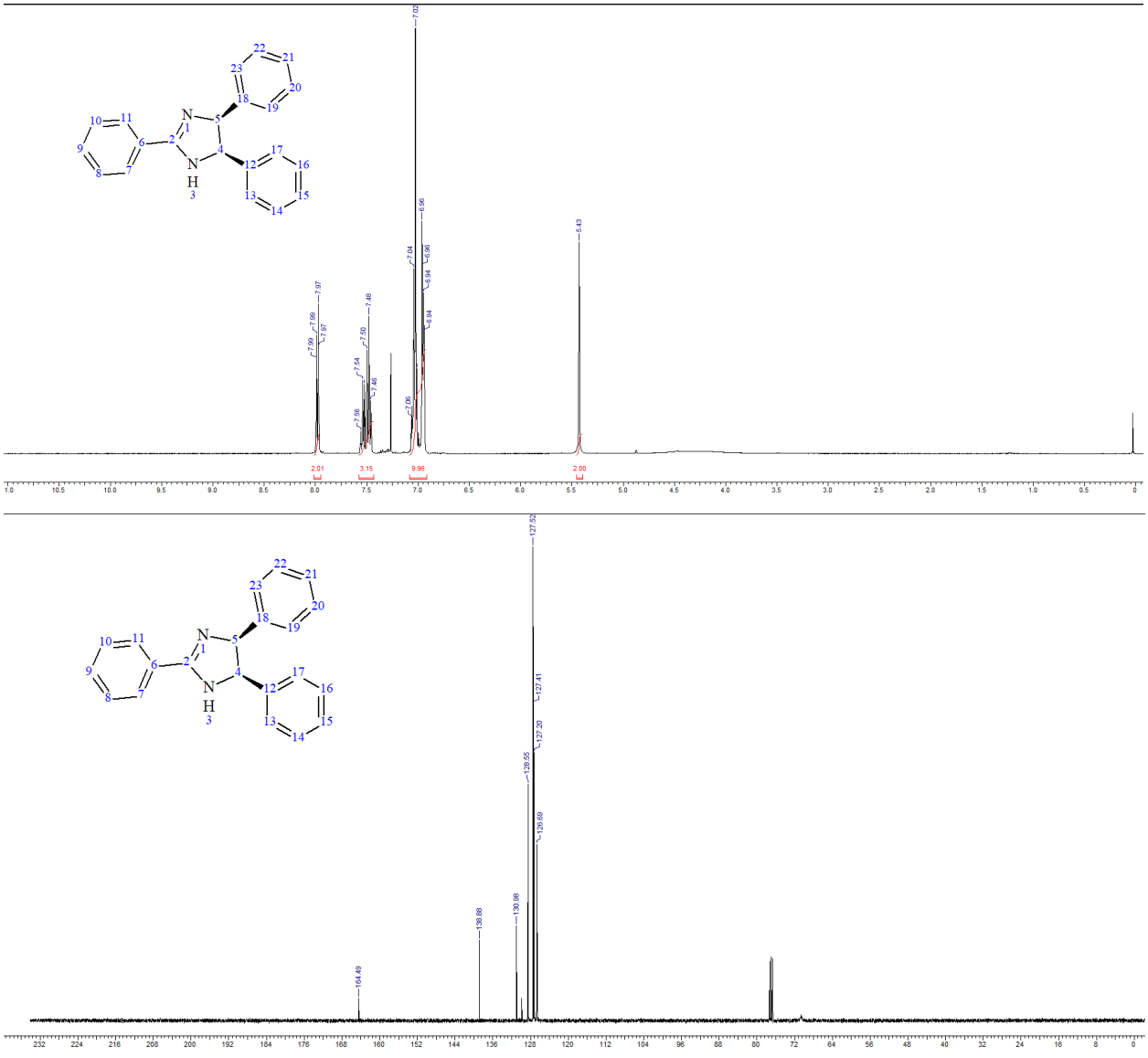
| Inhibitor | $k$, $\gamma$, $Z$ | Temperature, °C | | | | |
|---|---|---|---|---|---|---|
| | | 25 | 40 | 60 | 80 | 95 |
| - | $k$ | 5.7 | 17 | 105 | 620 | 1400 |
| 5 mM **4** | $k$ | 0.18 | 0.40 | 1.4 | 11 | 200 |
| | $\gamma$ | 32 | 43 | 75 | 56 | 7.0 |
| | $Z$ | 96.6 | 97.6 | 98.7 | 98.2 | 85.7 |
| 5 mM **4** + urotropine 25 mM | $k$ | - | - | 1.2 | 2.2 | 13 |
| | $\gamma$ | - | - | 88 | 280 | 110 |
| | $Z$ | - | - | 98.9 | 99.6 | 99.1 |
| 5 mM **5** | $k$ | 0.31 | 0.62 | 1.4 | 21 | 94 |
| | $\gamma$ | 18 | 27 | 75 | 30 | 15 |
| | $Z$ | 94.3 | 96.4 | 98.7 | 96.6 | 93.3 |
| **5** + urotropine 25 mM | $k$ | - | - | 1.2 | 3.2 | 8.7 |
| | $\gamma$ | - | - | 88 | 190 | 160 |
| | $Z$ | - | - | 98.9 | 99.5 | 99.4 |
| 5 mM **6** | $k$ | 0.51 | 0.99 | 2.4 | 230 | 1000 |
| | $\gamma$ | 11 | 17 | 44 | 2.7 | 1.4 |
| | $Z$ | 90.6 | 94.2 | 97.7 | 62.9 | 28.6 |
| **6** + urotropine 25 mM | $k$ | - | - | 2.2 | 2.5 | 11 |
| | $\gamma$ | - | - | 48 | 250 | 130 |
| | $Z$ | - | - | 97.9 | 99.6 | 99.2 |
| Urotropine 30 mM | $k$ | - | - | 7.8 | 43 | 200 |
| | $\gamma$ | - | - | 13 | 14 | 7.0 |
| | $Z$ | - | - | 92.6 | 93.1 | 85.7 |

**Synthethis**

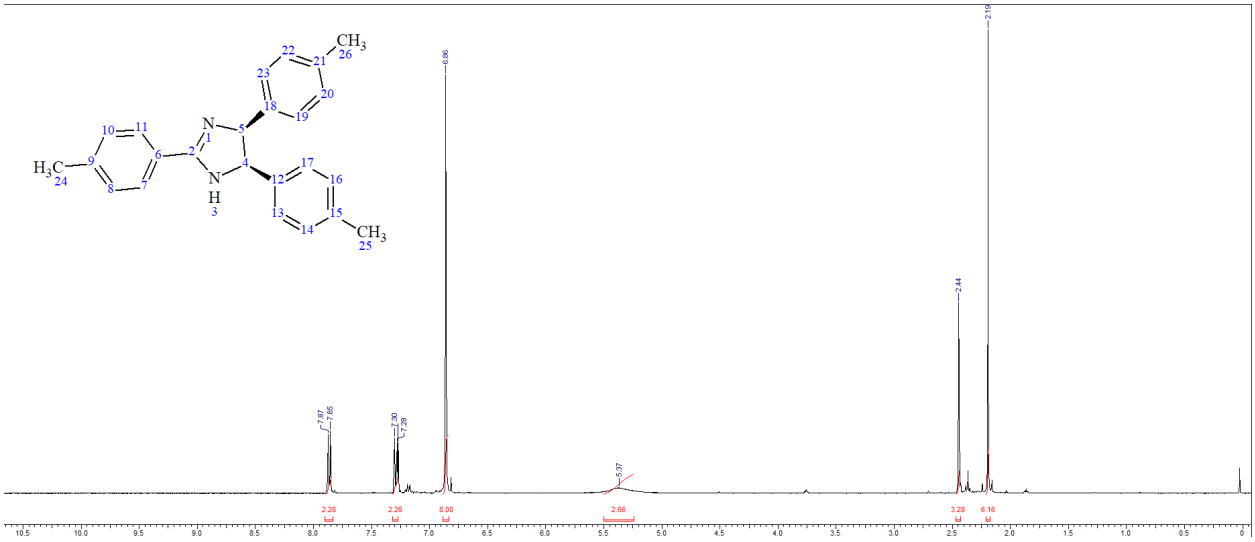
Compounds **4-6** were synthesized analogously to the procedure described for *cis*-imidazoline compounds as follows:

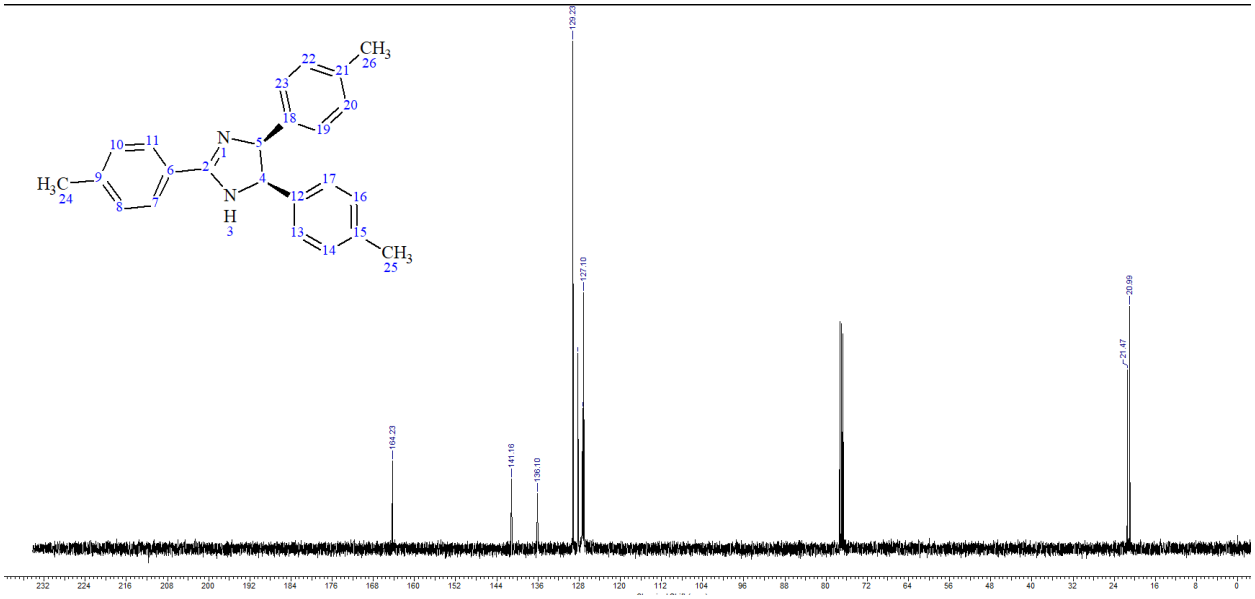
To 10 g of corresponding benzaldehyde in a beaker 200 g of aqueous ammonium (25%) was added. The obtained emulsion was stirred for 24 h at room temperature until all liquid of benzaldehyde was converted to 1,3,5-triaryl-2,4-diazapenta-1,3-diene as precipitate (for **4,5**) or as liquid (for **6**). The dried precipitates (or extract for **6**) was dissolved in 100 mL of THF or 1,3-dioxolane (distilled over sodium hydroxide). The solution was cooled in ice bath, and 3 g of potassium *tert*-butoxide was added on stirring. The solution became deep blue and after 0.5 min the color changed to yellow (in case of absence of dark color more potassium *tert*-butoxide should be added, the quantity depends on quality of THF). After color change, the solution was quenched with water (500 mL) and kept stirring in a open beaker for 12 h, until precipitate of product formed. The obtained precipitate was filtered, washed with water (100 mL), dried and used in experiments.

***cis*-2,4,5-Triphenyl-2-imidazoline (4)** $^{1}$H NMR (400 MHz, CDCl3): 5.43 (s, 2H), 6.94-7.06 (m, 10H), 7.46-7.56 (m, 3H), 7.97-7.99 (m, 2H). $^{13}$C NMR (400 MHz, $CDCl_3$): 126.69, 127.20, 127.41, 127.52, 128.55, 130.98, 138.88, 164.49.



***cis*-2,4,5-Tri-*p*-tolyl-2-imidazoline (5)** $^{1}$H NMR (400 MHz, $CDCl_3$): 2.19 (s, 6H ($2CH_3$)), 2.44 (s, 3H ($CH_3$)), 5.37 (s, 2H (2CH)), 6.86 (m, 8H (ArH)), 7.28 (d, J = 8.0, 2H (ArH)), 7.86 (d, J = 8.1, 2H (ArH)). $^{13}$C NMR (400 MHz, $CDCl_3$): 20.99, 21.47, 127.10, 127.34, 127.38, 128.26, 129.23, 136.10, 141.16, 164.23.





***cis*-2,4,5-Tris(4-isopropylphenyl)-2-imidazoline (6)** $^{1}$H NMR (400 MHz, CDCl3): 1.10 (d, J = 6.7, 12H), 1.32 (d, J = 7.0, 6H), 2.72 1.32 (p, J = 7.0, 2H), 3.00 1.32 (p, J = 7.0, 1H), 5.40 (s, 2H), 6.81-6.87 (m, 8H), 7.35 (d, J = 8.2, 2H), 7.91 (d, J = 8.2, 2H). $^{13}$C NMR (400 MHz, $CDCl_3$): 23.83, 23.95, 33.63, 34.13, 125.38, 126.65, 127.25, 127.32, 127.70, 147.29, 152.06, 164.18.