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## Experimental and theoretical studies of (*E*)-*N'*-1-(4-propylbenzylidene)nicotinohydrazide as corrosion inhibitor of mild steel in 1 M HCl

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## Abstract

The efficiency of a novel Schiff base namely (*E*)-*N'*-1-(4-propylbenzylidene)nicotinohydrazide (PBNH) was investigated as corrosion inhibitor of mild steel (MS) in 1M HCl using weight loss technique at 303 and 313 K. It was established that corrosion rate of mild steel increases with increase in temperature and concentration of HCl. Results showed that PBNH considerably inhibited the corrosion of mild steel in a 1 M HCl solution and inhibition efficiency is about 70% at  $4 \times 10^{-4}$  M PBNH at both temperatures. The inhibition efficiency of PBNH increased with an increase in concentration and temperature. The adsorption model obeys the Langmuir adsorption isotherm and the kinetic-thermodynamic model and the value of free energy of adsorption,  $\Delta_{Gads}$  indicated that the adsorption of PBNH was a spontaneous process and was both an electrostatic-adsorption (physisorption) and adsorption on the basis of donor-acceptor interactions (chemisorption). Thermodynamic parameters calculated show the spontaneity and endothermic nature of the process and also reveal the favourable affinity of PBNH towards the mild steel surface. Quantum chemical calculations based on PM3 method was performed on PBNH and calculated parameters gave useful information to explain the interaction between the surface of metal and PBNH.

The article is published in the original.

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