

Structural Effects and Mechanism of the Inhibition of Acid Corrosion of Steel by Some dithiocarbamate derivatives.

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Barriers to internal rotation around the C-N bond have been calculated for the isoelectronic series N-formylpyrroole, N-formylimidazole and N-formylpyrazole at their optimized geometries . The magnitudes and origins of the calculated barriers have been discussed in terms of energy partitioning analysis. The major source of barriers in the studied molecules is predicted to be due to the bonded overlap interactions across the C-N bonds.

Exchange and electrostatic interactions are found to be important for rotation angles in the range  $35^\circ > \theta > 120^\circ$ .