

عنوان مقاله:

INVESTIGATION OF THE EFFECT OF MOLECULAR STRUCTURE ON CORROSION INHIBITION FOR SOME ORGANIC COMPOUNDS

محل انتشار:

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تعداد صفحات اصل مقاله: 5

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خلاصه مقاله:

The effect of some organic compounds with C=N and OH groups on the inhibition efficiency for corrosion of metal has been investigated by some theoretical methods. The molecular orbital calculations explain the adsorption of the inhibitors to the surface through the C=N and OH centers which may be due to the lengthening of the C=N and OH bond lengths and the increasing of electron density on the nitrogen and oxygen atoms. The calculations explain that the presence of electrophilic group shows the highest charge density on the nitrogen and oxygen atoms and the highest protection efficiency due to its polar interaction with a metal surface.

کلمات کلیدی:

Anti corrosion, electrophil group, Theoretical investigation, Molecular structure

لینک ثابت مقاله در پایگاه سیویلیکا:

<https://civilica.com/doc/22300>

