عنوان مقاله:

Study of the corrosion inhibition efficiencies some amino Acids by quantum chemical calculations

محل انتشار:

اولین همایش ملی فناوری های نوین در صنایع نفت و گاز (سال: 1389)

تعداد صفحات اصل مقاله: 9

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خلاصه مقاله:

Quantum chemical calculations using the density functional theory (DFT) and ab initio methods were performed on nine amino acids grouped under three skeletons used as corrosion inhibitors for mild steel to determine the relationship between molecular structure and their inhibition efficiencies.the results of the quantum chemical calculations and experimental %IE were subjected to correlation analysis and indicate that their inhibition effect are closely related to hardness, polarizability, electrophilicity. The %IE increased with increase in plarizability, electrophilicity and decrease in hardness

کلمات کلیدی:

(plarizability, electrophilicity, hardness, inhibition efficiencies(IE), density functional theory(DFT