

# Substituent effects in frontier orbitals of cyclic hydroxamic acids

Weiss-López, Boris

Bravo, Héctor R.

AM1 full geometry optimization of seven substituted cyclic hydroxamic acids (Hx) was performed. A qualitative correlation between Elumo vs Hammett's  $\rho$ P was observed. The reactivity of these 7-substituted Hx with hard nucleophiles seems to follow basic principles of frontier orbitals theory. Experimental support was obtained from the reaction of six Hx with 2-methoxyethylamine. © 1994.