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Theoretical study of charge transfer complexes between antithyroid thioamides and TCNE: Thermodynamics of the complex formation

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Abstract

Thermodynamic characteristics of charge transfer complexes formed between both mono and bicyclic thioamides as donors and tetracyanoethylene have been studied by selected Density Functional Theory and Wave-Function based methods combined with the Polarizable Continuum Model. The thioamide derivatives are known to exhibit significant antithyroid activity. The equilibrium constants of complex formation (K) derived from calculated thermodynamic parameters nicely correlate with the donor strength while their experimental counterparts reveal practically no correlation. Based on theoretical calculations we conclude that the rather erratic behaviour of the experimental K values is related to the presence of chemical reactions including radical ions formation, which proceed along with the π -complex formation.

Keywords: Thioamide; Charge transfer complex; Thermodynamic; Density functional methods

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