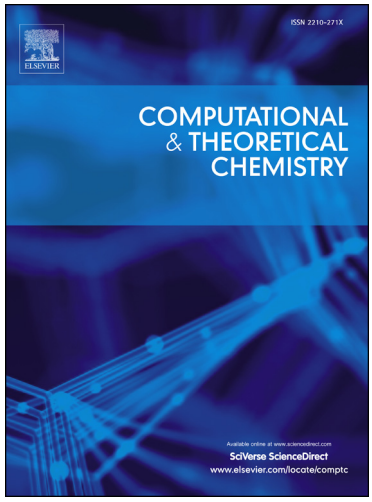


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# Theoretical study of charge transfer complexes between antithyroid thioamides and TCNE: Thermodynamics of the complex formation

**Šimon Budzák,[1*] Pavel Mach,[2] György Juhász,[3] Miroslav Medveď,[1] Ondrej Kyseľ[1]**

[1]*Department of Chemistry, Faculty of Natural Sciences, Matej Bel University, Tajovského 40, SK-97400 Banská Bystrica, Slovak Republic, simon.budzak@umb.sk, miroslav.medved@umb.sk, ondrej.kysel@umb.sk*

[2]*Department of nuclear physics and biophysics, Faculty of Mathematics, Physics and Informatics, Comenius University, Mlynská dolina F1, SK-842 48 Bratislava, Slovak Republic, pavel.mach@fmph.uniba.sk*

[3]*Department of Chemistry, Faculty of Education, Janos Selye University, Bratislavská cesta 3322, SK-94501 Komarno, Slovak Republic, juhaszg@ujs.sk*

*corresponding author, telephone number +421 48 446 7348

## 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