ABSTRACT


Coordination compounds of dialkyldithiocarbamate have broad applications, e.g. automotive lubricant additives. Coordinated long chain dialkyldithiocarbamate was studied to obtain the better anti-friction and anti-wear. Integration of computation chemistry e.g. density functional theory used to identify reaction mechanisms, to optimize geometry of structure, and to estimate properties of compounds. The aim of this study was to obtain long chain complexes Zn-dialkyldithiocarbamate, to examine their structures, and to estimate their applications using Density Functional Theory methods (DFT). Long chain dialkyldithiocarbamate was synthesized through reaction between ZnCl₂, OH, CS₂ and secondary amine during 24 hours in room condition. Secondary amine was obtained from LiAlH₄ reduction of amide during 24 hours in nitrogen atmospheric. Reaction of long chain amine and long chain acylchloride was used to obtain amide. DFT and instrumentation (FTIR and HPLC) was used to study of mechanism, structure elucidation and its application. The results showed the synthesis of Zn-dibutyldithiocarbamate, dipalmitilamide, dipalmitilamine, Zn-dipalmitildithiocarbamate yields are 90.02%, 90.91%, 47.5%, and 66.49% respectively. The ratio of intensity and wave number for Zn-dibutyldithiocarbamate from FTIR spectra and DFT calculations wasn’t significantly different at 95% confidence level. According to DFT calculation (B3LYP/ 6-31G*), the carbon-sulfur bonds in Zn-dibutyldithiocarbamate have an average length of 0.1683-0.1743 nm and the ligand “bite” angle S-C-S has a mean value of 116.85°. This result indicates a tetrahedral-shaped Zn-dibutyldithiocarbamate. Lubricant additives (anti-wear and anti-friction) properties of Zn-dialkyldithiocarbamates was estimated by chemical hardness and absolute electronegativity. Lower electronegativity value is better anti-friction, and lower chemical hardness is better anti-wear. Anti-friction ability of Zn-dialkyldithiocarbamate is better than Mo-dialkyldithiocarbamate, while anti-wear ability is lower than Zn-dialkyldithiophosphates. Based on electronegativity absolute value of DFT calculations, the Zn-dialkyldithiocarbamate is categorized superlubricity that can perform in the boundary lubricant system.

Key word: DFT, Zn-dialkyldithiocarbamate, chemical hardness, absolute electronegativity, anti-wear, anti-friction