**ABSTRACT**

The Structure And Electronic Properties Of Dihydrogen Bond Complexes That Form Between H Of M-H (Where M-H=Lih, Nah, Kh, Feh2, And Znh2) And H Of Acetylene Hc≡ Chand H Of Ethylene Hch=Hch Compounds Was Predicted Employing Density Functional Theory. The Ground State Dihydrogen Bond Complexes Were Optimized At B3lyp-6-311++G\*\* Level Of Theory. The Geometrical Parameters, Energies, Entropies, And Aim Analysis Of The Considered Complexes Were Calculated And Analyzed.