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Comparison of structural parameters in antiparkinson's drug: Procyclidine & its nano carrier based on fullerene with calculation chemistry

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Abstract

Parkinson's disease is a degenerative disorder of the central nervous system. It results from the death of dopamine-containing cells in the substantia nigra, a region of the midbrain; the cause of cell-death is unknown. Procyclidine is used to treat parkinsonism (slowed movements, stiffness of the body, uncontrollable body movements, weakness, tiredness, soft voice, and other symptoms caused by damaged nerves in the brain). Procyclidine is also used to treat problems with moving and drooling that may be caused by certain medications for mental illness. Procyclidine is in a class of medications called antispasmodics or antimuscarinics. It works by preventing sudden tightening of the muscles. In this Study at the first compounds $[C_{60}$- Procyclidine–Cn-2X$]^+$ and [Procyclidine-Cn-2X$]^+$ (X=F,Cl,Br) were optimized (n is similar to in two compound). All calculations is done in 6-31g* basis set in HF method and in gas phase. The results showed that the energy levels of molecular orbital (HOMO & LUMO) in the RF has the lowest value. C_{62}-X, C_{62}-N_{61} has a length of the shortest bond and the bond has most power. Comparison of the dipole moments of compounds shows this trend: R-2Br > R-2Cl> R-2F.This is noticeable that the trends in these compounds are quite similar but the values in only drug are more intense than drug with fullerene.

Keywords: Procyclidine, Parkinson , nano carrier, fullerene

1. Introduction