

Abstract Submitted
for the MAS20 Meeting of
The American Physical Society

Study on the Boron Derivatives for Tumor Cell Treatment Using Stereochemical Analysis SUNGWON CHUNG, RICHARD KYUNG, CRG-NJ — Boron Neutron Capture Therapy (BNCT) is an emerging science as a tool in treating cancer. This paper explains the novel structures and stabilities of the boranes based on the molecular orbital theory. A common application for the boranes is the process of hydroboration resulting in the formation of organoboranes. They are important for a potential treatment for cancer known as Neutron Capture Therapy. In this paper, physicochemical effects of commercially used boranes were analyzed using computational simulations. The molecules were observed and analyzed using density functional theory. Such compounds can selectively kill affected cells without being toxic to non-affected cells. Electrostatic potential maps were also used to interpret the activity of the molecules. Molecular editing software was used to measure the optimization energy and the dipole moment of each molecule. Data shows the Octahydrotriborate is very stable and it has a higher boron to hydrogen ratio so that it can deliver more boron to the cancer affected site to perform Neutron Capture Therapy.

Richard Kyung
CRG-NJ

Date submitted: 02 Nov 2020

Electronic form version 1.4