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Thermodynamic and Stereo-chemical Analysis of Gadolinium and Iodinated Contrast Agents for Diagnosis of Alzheimer's Disease YOOSONG SONG, RICHARD KYUNG, Choice Research Group — Gadolinium derivatives have become commonly used for Contrast Agents in medical treatments such as early diagnosis of Alzheimer's disease. The unique magnetic properties of the gadolinium ion allowed it to be used in a variety of ways, especially in MRI scanning. The energy optimization feature of the Avogadro, Chemcraft and Gaussian programs allow evaluation of the molecules thermodynamic and biomedical stability and efficiency. In this paper, the thermodynamic and stereo-chemical effectiveness of gadolinium-based molecules as MRI contrast agents was analyzed. The PC61BA-(Gd-DO3A), a functionalized fullerene that is created through synthesis of PC61BA and Gd-DO3A was modeled and analyzed. Also functionalized polymers with highly iodinated molecules were studied. By making efficient use of the computational programs, we were able to study the computational and theoretical aspects of the functionalized Gadolinium molecules and iodinated molecules to determine whether the derivatives are safe and stable contrast agents. The Auto Optimize Tool and Universal Force Field (UFF) options were used for each and every derivatives modeled in this project to determine its optimization energy.

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