عنوان مقاله:

DFT Study of PAMAM dendrimers as drug delivery vehicles for platinum anticancer drugs

محل انتشار:

اولین همایش ملی تکنولوژی های نوین در شیمی و پتروشیمی (سال: 1393)

تعداد صفحات اصل مقاله: 3

نویسندگان:

d Farmanzadeh - *Department of Physical Chemistry, Faculty of Chemistry, University of Mazandaran,Babolsar. Iran*

m Ghaderi - *Department of Physical Chemistry, Faculty of Chemistry, University of Mazandaran,Babolsar. Iran*

خلاصه مقاله:

It is a great challenge for nanomedicine to develop novel dendrimers with maximum therapeutic potential and minimum side-effects for drug and gene delivery. As delivery vectors, dendrimers must overcome lots of barriers before delivering the bio-agents to the target in the cell. Quantum mechanical studies can be used to accurately understand the interactions between dendrimers and molecules of pharmaceutical and industrial interest. In this study, we implemented a density functional theory to calculate the interaction energy zero generation (G0) of Polyamidoamine (Pamam) dendrimer with picoplatin(ZD) anti-cancer drug with three active sites (Clα,Clβ, NH3) at the B3LYP level. In order to better understand the surface loading and distribution of picoplatin molecules, molecular reactivity was determined by evaluation of electronic properties. It was shown that G0–ZD (NH3) has greater electron transfer and hence, a stronger interaction than other one.

کلمات کلیدی:

Polyamidoamine (PAMAM) dendrimer, Picoplatin, Density Functional Theory, Electronic Properties