عنوان مقاله:

The boron-fullerene nanocage as an effective carrier for the delivery of cyclophosphamide and its derivatives: A DFT study

محل انتشار:

اولین همایش بین المللی افق های نوین در علوم پایه و فنی و مهندسی (سال: 1395)

تعداد صفحات اصل مقاله: 7

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خلاصه مقاله:

The structures of boron-doped fullerene B-C59 (1) as a drug delivery system, two derivatives of cyclophosphamide anticancer prodrug (2 and 3) as well as their covalently bonded structures 4 and 5 were optimized by DFT computations at B3LYP level of theory using 6-31G(d) basis set. Comparing compounds 4 and 5 revealed that the bromo derivative (-22.5569 kcal/mol) was more stable than its chloro analogue (-22.0483 kcal/mol). The dipole moments of isolated drugs (~ 5.2, 5.1 D) had almost half values compared with those of their related compounds covalently bonded to the B-C59 (~ 9.7, 9.8 D) reflecting attachment of drugs on the B-C59 significantly enhanced the polarity of the whole systems which was a desired property for drug delivery in biological media. The HOMO-LUMO band gaps of pristine B-C59 (1) and isolated drugs 2, 3 were near 2.3 and 2.7 eV, respectively while those of compounds 4, 5 were smaller (2.1 eV) indicating decrease in electrical conductivities of the isolated drugs/B-C59 upon interactions.

کلمات کلیدی:

DFT computation, Cyclophosphamide, Drug delivery, B-C59 nanocage, band gap

لینک ثابت مقاله در پایگاه سیویلیکا: