β-βCyclodextrin Interaction with Edaravone: Molecular Modeling Study

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Résumé

PM3 DFT, HF, and ONIOM2 calculations were performed on the inclusion complexation of β-cyclodextrin with edaravone (EDA). The results obtained with PM3 clearly indicate that the complexes formed are energetically driven; the B orientation (EDA entering into the cavity of β-CD from its wide side) is found stabler than the A orientation (EDA entering into the cavity of β-CD from its narrow side). The structures show several intermolecular hydrogen bond interactions that were studied on the basis of NBO analysis used to quantify the donor–acceptor interactions between the guest molecules and β-CD.

Mots-Clés: β, CD, Edaravone, PM3, DFT, HF, ONIOM2, NBO, Inclusion complexation

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