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Possibility of using hetero-derivatives of fullerene C60 as the carriers of drugs containing benzene, naphthalene or anthracene ring - endohedral complexes @C54Y6

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Statement of the Problem: The effects of the aromatic compounds on the boron, silicon and sulphur, fullerene C60 hetero-derivatives stability and possibility of using created endohedral heterofullerenes as the carriers of compounds with pharmacological activity.

Methodology: All endohedral complexes were created by substitution of six carbon atoms of the fullerene cage by boron, silicon or sulphur atoms and all the heteroatoms were placed in the same hexagonal ring. The following complexes were studied: C6H6@C54B6, C6H6@C54Si6, C6H6@C54S6 C10H8@C54B6, C10H8@C54Si6, C10H8@C54S6, C14H10@C54B6, C14H10@C54Si6 and C14H10@C54S6. After geometry optimization of each compound examined, all the lowest energy conformers were placed into carbon cages created of heterofullerene C60 each and geometry of each complex was optimized. The energies of stabilization (Estab.), deformation (Edef) as well as total energy (E) of each examined heterofullerenes C60 and their complexes (Ecx) with benzene, naphthalene and anthracene were calculated with the use of the molecular modeling technique (HF with STO-3G basis set, Spartan '14 software).

Findings: There were slight changes in the shape of the structure C6H6@C54B6 and very visible structural disturbances in C10H8@C54B6, C14H10@C54B6. The flat molecules of naphthalene and anthracene were strongly distorted. The shape of the C6H6@C54S6, C6H6@C54Si6 and C14H10@C54Si6 structure is similar to a "barrel" but in C10H8@C54Si6 and C14H10@C54S6 complexes, six-membered heteroatom rings were very stretched and deformed. In case of C10H8@C54S6 significantly elongation of six-membered heteroatom ring results in naphthalene release. The results reveal that examined systems are thermodynamically unstable However; calculation suggests that those systems could exist despite positive energy values and therefore the possibility of using them as drug carriers may be assumed.

Conclusion: The tendency for some kind of ring opening may indicate the direction for further drug nanocarriers research and their opening ability to release compounds with pharmacological activity in the proper molecular target.

Recent Publications:

1. Matsubara M and Massobrio C (2007) Charge effects in silicon-doped heterofullerenes. Applied Physics A 86(3):289–292.
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Biography

Monika K Grudzień completed her PhD in 2010 and it was rewarded in 2011. She is the Associate Professor at Department of Drug Chemistry, Faculty of Pharmacy with the Laboratory Medicine Division Medical University of Warsaw.

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