



Structure, stability, aromaticity of C_{20-n}S_n heterofullerenes(n=0-10)

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Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | Since the discovery of the "buckyball" (fullerene C₆₀) in 1985 as a stable allotrope of carbon with a closed cage structure and then macroscopic scale synthesis of C₆₀, fullerenes have attracted great scientific interest for their possible applications especially as nanomaterial and biomedical species. It was found that fullerenes and their derivatives possess diverse medical applications and are promising as HIV inhibitor, photosensitive oxidizing agents against malignant skin cancer, Magnetic Resonance Imaging contrast agents, gene or drug delivery carriers and neuroprotection by antioxidant activity for healing neurodegenerative illnesses. Here, the ideal goal of substitutional doping of fullerene cage is to improve its characteristics for special purposes while keeping its structural stability. Based on Hoffmann, Schleyer and Schaefer's statements on colloquial use in chemistry "stability" is 95% kinetic, 5% thermodynamic. In physics, it's just the opposite. Hence, DFT calculations are applied to compare and contrast of substitution effects on structural, thermodynamic stability and kinetic stability of heterofullerenes. Computational surveys are waiting experimental testing. | Format: Paperback | Language/Sprache: english | 64 pp.



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