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DFT calculation of non-linear optical properties of 2,5,8,11,14,17-hexa-tert-butyl-hexa-peri-hexabenzocoronene molecule and its derivative molecule functionalized with one potassium atom: influence of doping

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Introduction

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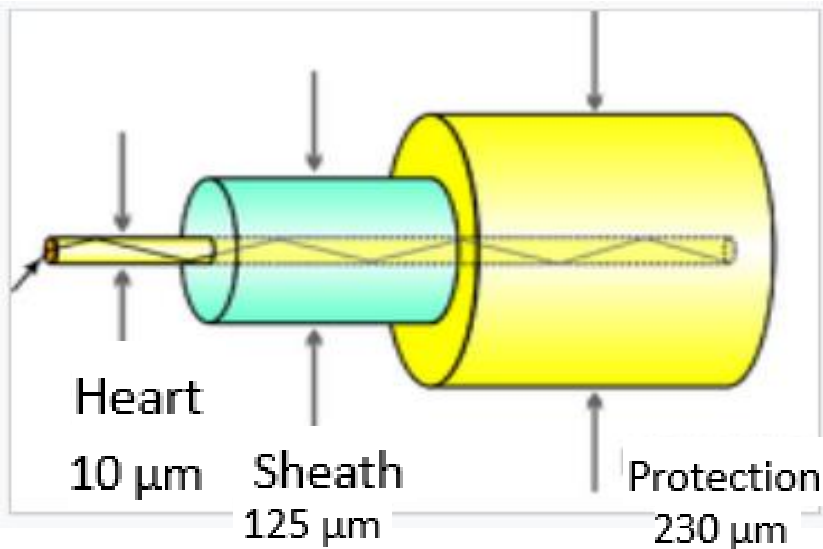


Figure1: Component of an optical fiber



Improvement of materials at the level of the optical fiber

- Materials with a good absorption spectrum in the visible range
- Materials with a high value of first-order hyperpolarizability

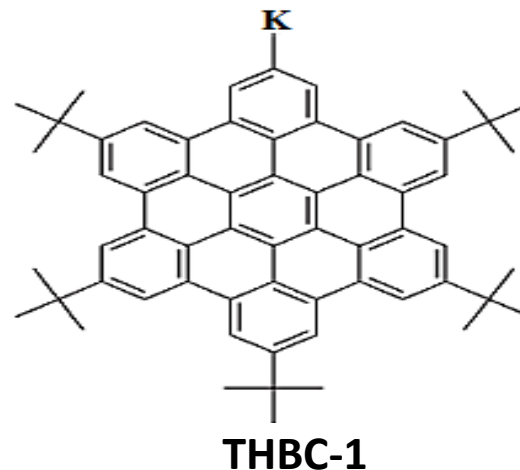
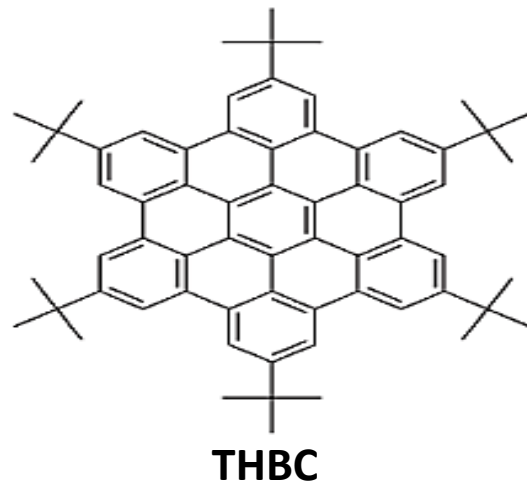


Figure 2: 2,5,8,11,14,17-hexa-tert-butyl-hexa-peri-hexabenzocoronene molecule (first left) and its derivatives molecules functionalized with one potassium atom (second right)

Introduction

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Purpose of our research is

Extend the field of application of the 2,5,8,11,14,17-hexa-tert-butyl-hexa-peri-hexabenzocoronene molecule in the field of nonlinear optics

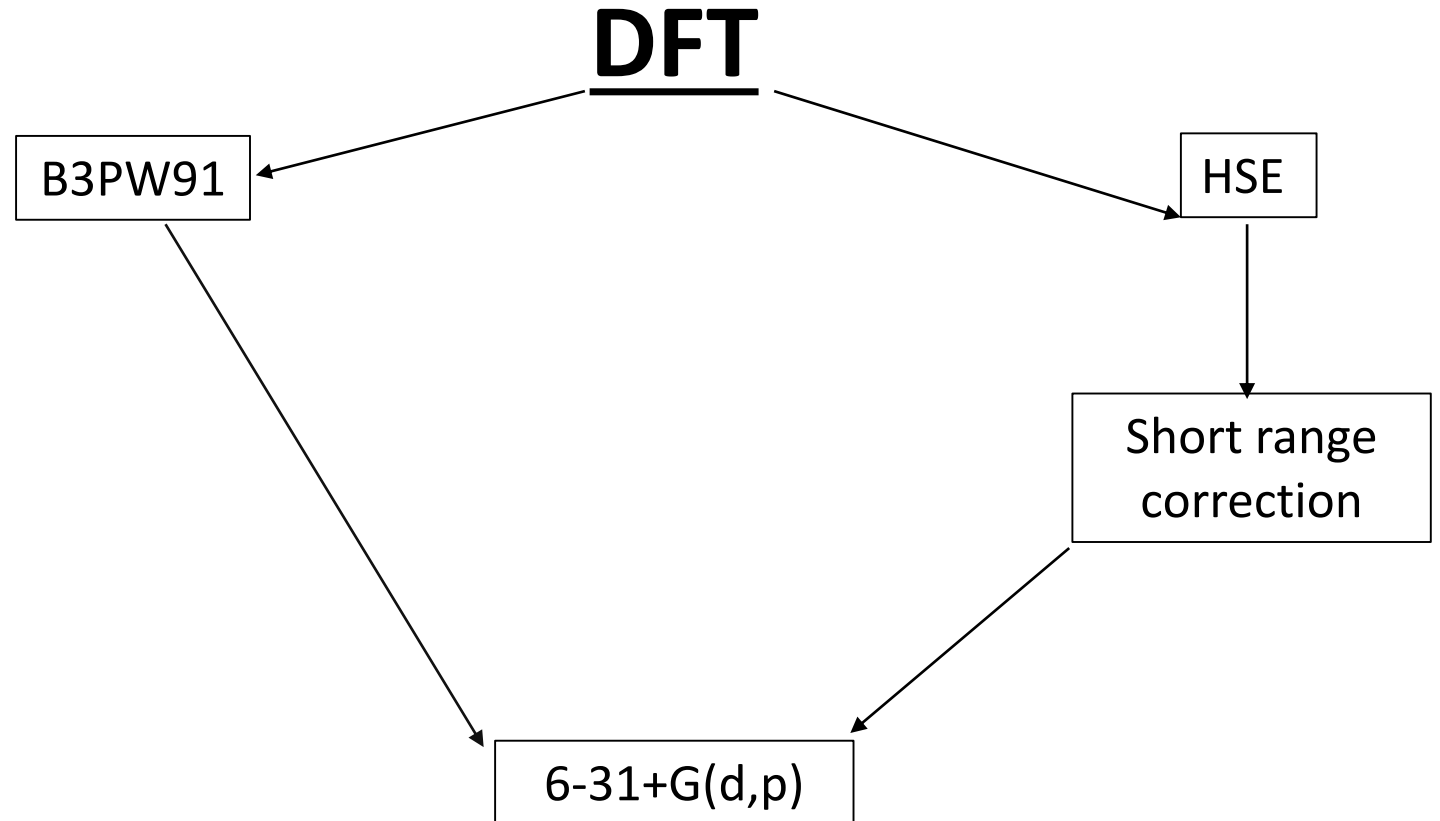
Main objective

Improve the properties of the 2,5,8,11,14,17-hexa-tert-butyl-hexa-peri-hexabenzocoronene molecule through its derivatives doped with the potassium atom

Methods & material

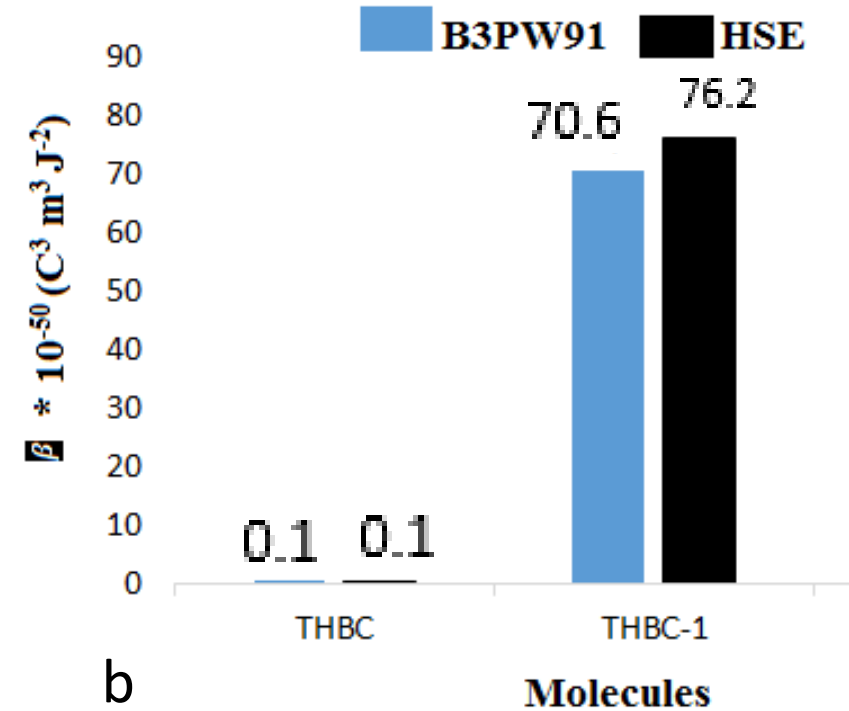
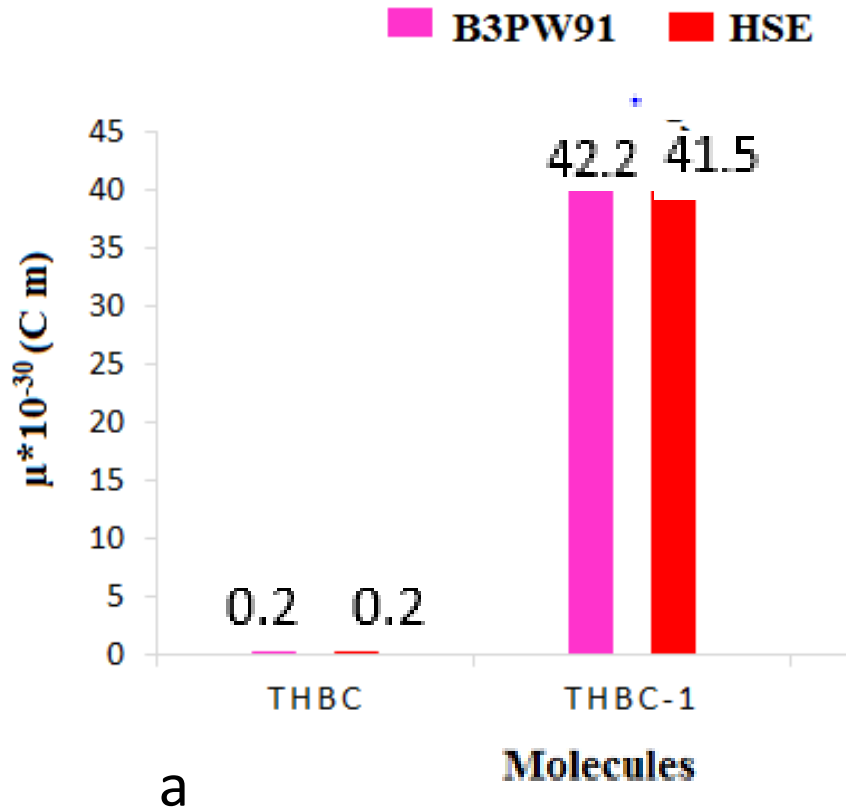
Material

- GaussView
- Gaussian 16
- Matlab 2014



Nonlinear optical properties

$$\beta_{\text{PNA}} = 343.7 \cdot 10^{-52} \text{ C}^2 \text{ m}^2 \text{ j}^{-2}$$



Dipole moment (μ) and first-order hyperpolarizability (β)

Conclusion