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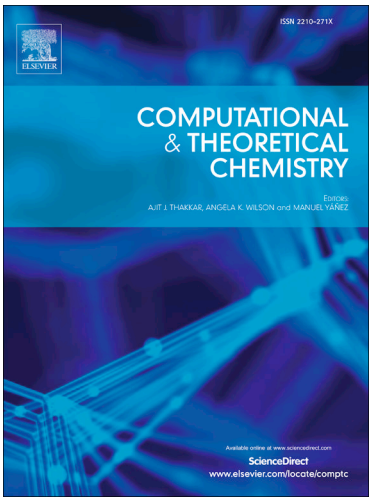

Tris(perfluoroalkyl)germylethynyl derivatives of biphenyl containing ferrocenyl donor group: structure, spectra, and photoinduced intramolecular electron transfer

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PII: S2210-271X(17)30477-2
DOI: https://doi.org/10.1016/j.comptc.2017.11.007
Reference: COMPTC 2664

To appear in: *Computational & Theoretical Chemistry*

Received Date: 31 July 2017
Revised Date: 27 October 2017
Accepted Date: 6 November 2017

Please cite this article as: E.P. Chuhmanov, N.L. Ermolaev, B.N. Plakhutin, S.K. Ignatov, Tris(perfluoroalkyl)germylethynyl derivatives of biphenyl containing ferrocenyl donor group: structure, spectra, and photoinduced intramolecular electron transfer, *Computational & Theoretical Chemistry* (2017), doi: https://doi.org/10.1016/j.comptc.2017.11.007

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ACCEPTED MANUSCRIPT

Tris(perfluoroalkyl)germylethynyl derivatives of biphenyl containing ferrocenyl donor group: structure, spectra, and photoinduced intramolecular electron transfer

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Ferrocenyl derivatives with perfluorinated organometallic fragments are prospective sensitizers for photovoltaic devices which can provide higher stability and resistance to oxidation in comparison with the known analogs. For the development of the photovoltaic devices based on such molecules, the estimates of probabilities of photoinduced electron transfer both inside the molecule and from the molecule to the internal semiconductor electrode are required. In this work, the structural, electronic, spectral and radiative parameters of trialkylgermyl (alkyl = Me, *n*-C_3H_7, CF_3, *n*-C_3F_7) derivatives of 4,4'-diethynylbiphenyl containing ferrocenyl donor group are considered. The spectral and radiative parameters of these compounds were calculated using the TD-DFT theory with the B3LYP, PBE0, BHandHLYP и CAM-B3LYP functionals. For all the molecules, the probabilities of photoinduced electron transfer to the outer molecular fragments inside the sensitizer are estimated on the basis of direct analysis of charge redistributions in the excited states.

Keywords: ferrocene, germanium, photoinduced electron redistribution, DFT

1. Introduction

The insertion of electron-acceptor groups into a conjugated structure is a well-known method of the organic *n*-type semiconductors formation [1-6] suitable, for example, for the development of photovoltaic devices. This method provides the broad variation of the formed material properties depending on the type of substituents. For such purposes, the perfluorinated aliphatic [7-9] or the organoelement [10-12] substituents are used frequently. In our previous study [13], we used the powerful electron-withdrawing $(CF_3)_3Ge$ group in order to analyze its impact on aromatic π-conjugated systems. It was found that the perfluoroalkyl substituents results in the appearing of excited states with the high intramolecular charge transfer to a heteroatom. Earlier, it was demonstrated that the formed compounds are characterized by the increased durability and resistance against the environmental factors [14].

Some structures studied in [13] were formed by the electron-acceptor $(CF_3)_3Ge$ group connected with 4-ethynylbiphenyl moiety. This compound had the lowest observed fluorescence decay rate and high quantum yield of observed charge transfer which make it a prospective candidate for photovoltaic materials. At the same time, the influence of the fluorinated substituent variation was not studied. Such variation is rather impractical in experimental studies due to the difficult synthesis of fluorinated organoelement compounds. Therefore, in the current work, we study the influence of the fluorinated substituents on the electronic properties of potential candidate molecules using the quantum chemical calculations. The main goal of this study is the determination how the combination of ferrocenyl radical, as an electron donor, and the organogermanium perfluorinated group, as a

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