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MODELING OF BRANCHED FLUORENYLIDENE DERIVATIVES. STRUCTURE AND ENERGETICS USING QUANTUM CHEMISTRY APPROACH

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Abstract
Quantum chemical study of several HTMs compounds is presented and discussed. Problems of the ground state geometry optimizations and excited state geometry optimizations were evaluated through matching the simulated results with the experimental ones.
Key words: *quantum chemical study, HTMs.*

1. Introduction

Organic perovskites represent a promising class of materials with the potential to revolutionize various aspects of energy conversion and optoelectronics [1] as efficient and flexible photovoltaic materials. Organic perovskite solar cells have shown remarkable progress in efficiency, reaching levels comparable to traditional silicon-based solar cells [2]. Due to long carrier diffusion lengths and high light absorption coefficient, usage of organic perovskites can open new possibilities for even more advanced technologies.

This work is devoted to the quantum chemical study of several HTMs [3]. Structure of 9-(4-bis(4-((2,7-bis((9-9-ethyl-9*H*-carbazol-3-yl)(4-ethoxyphenyl) amino)-9*H*-fluoren-9-ylidene)methyl)phenyl)amino)benzylidene-N^2,N^7-bis (4-methoxyphenyl)-9*H*-fluorene-2,7-diamine (V1389) is presented in Fig. 1.

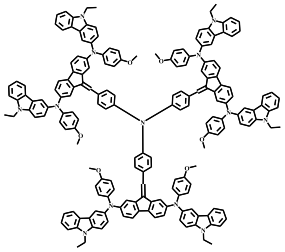


Fig. 1. V1389

2. Review of research

Simulations of the ground state molecular structures for several of the most probable conformers were provided using Gaussian 16 software [4] using density functional theory (DFT) B3LYP method and 6-31G(d) basis set, supplemented with polarization functions (d). Fig. 2 represents molecular structure of two conformers V1389 after ground state energy optimization routine. All presented structures were obtained using grad optimization technique (convergence of parameters Maximum Force, RMS Force, Maximum Displacement, RMS Displacement has been achieved). Electronic excitations were simulated using the semi-empirical TD method (for singlets). Spatial distribution of the electron density for the HOMO−1, HOMO, LUMO, and LUMO+1 was analysed – see Table 1. For V1389, central unit is formed from three phenyls related through nitrogen atom. Charge redistribution between left and right substituents and central core is established for both conformers, a and b.

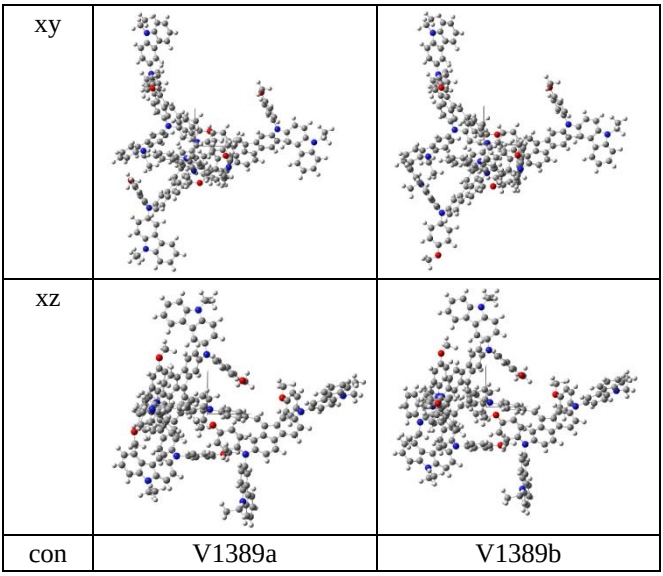
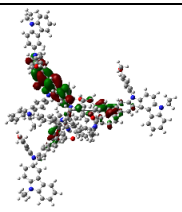
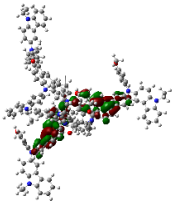
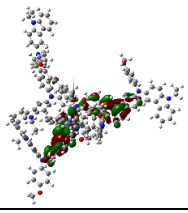
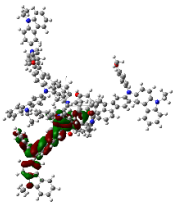
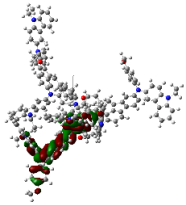
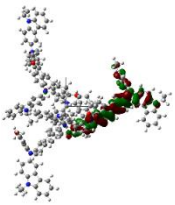
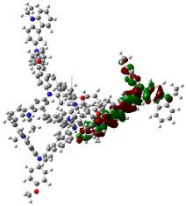
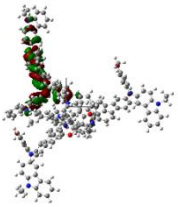
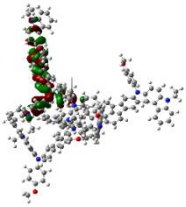


Fig. 2. Molecular structure of two conformers V1389 after ground state energy optimization routine using *Gaussian16*, B3LYP/6-31G(d) basis set

Table 1

Compounds V1388 and V1389. Set of MO involved into "spectroscopic" states $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$

MO	V1389a	V1389b
LUMO+1		
LUMO		
HOMO		
HOMO-1		
HOMO-2		

3. Conclusions

HTMs molecules exhibit charge transfer behaviour in partially in-plane/in-plane or twisted excited-state geometries that strongly depend on environmental parameters.

Acknowledgments

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