

# New Co-Oligomers involving Polyvinylcarbazole (PVK) and Pyrrole for Organic Solar Cells Applications Structure/Properties Correlation by Density Functional Theory (DFT) Study

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## Abstract

*In this paper, we have used the DFT for study a new copolymer based on Poly(vinyl)carbazole (PVK) and Pyrrole (Py) to investigate polymers with precisely defined molecular architecture and to better explore, we suggest in this work theoretical research supported by experimental results of the synthesis and properties of this copolymer. The wish is to suggest an oligomer model that reflect properties of copolymer. Subsequently, we have used these quantum chemical calculations to supply a complete characterization of the molecular geometry, electronic structure, and spectroscopic characteristics of this oligo-mer. We have determined the photovoltaic properties to test the possibility of proposing this oligomer or the corresponding copolymer for applications in the field of organic solar cells.*

**Keywords:** Polyvinylcarbazole (PVK), Density Functional Theory (DFT) Calculations, Copolymerization Mechanism

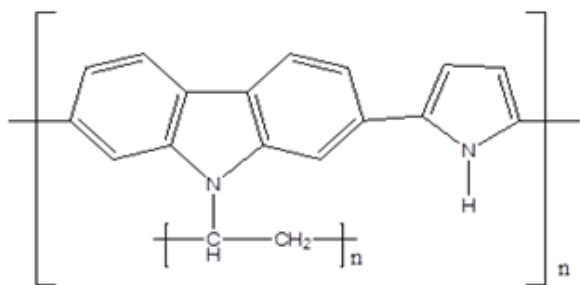
## Introduction

Polymers with carbazole groups such as polyvinylcarbazole were largely investigated because of their photoconductivity, photoluminescence, and hole transport properties [1,2]. Polyvinylcarbazole has attracted attention in applications related to organic light emitting diodes (OLED) [3]. It is one of the most important polymeric materials as it has many applications in industry and is relatively cheaper. Its unique chemical and physical properties led to its wider applicability. Also, Polyvinylcarbazole have amply used for electronic display, many electrical & electronic devices and home appliances [3,4]. Due to its high tensile strength and good abrasion resistance, Polyvinylcarbazole is used in double layer capacitors and electrochemical windows etc [5]. Trends of organic EL devices based on Polyvinylcarbazole have been focused both on optimizations of EL structure and developing new materials [6]. Different types of EL structures have been proposed [7]. There still existing demand for searching more efficient material with the simplified

architecture. On the other hand, Pyrrole (Py) is a heterocyclic aromatic organic compound comprising a five-membered ring used as precursors to prepare thousands of organic compounds that will serve for diverse applications [8]. Among these compounds, polypyrrole, which possesses high electrical conductivity, environmental stability, and biocompatibility and many, interesting electronic properties. These latter have made it possible to propose this material for applications such as chemical and electrochemical sensors in electronic and optical devices, electrochromic devices, actuators and field emission applications [9]. The new copolymer Polyvinylcarbazole (PVK)-(pyrrole) has an interesting properties compared to PVK and pyrrole homopolymers taken separately. We hope that the present results could help to clarify whether the structure of the neutral copolymer as suggested by experimental results, which would then be exploited in organic electronics [10]. We propose in this work, theoretical research supported by experimental results of the synthesis and properties of a new copoly-

mer based on Polyvinylcarbazole (PVK) and Pyrrole (Py). This copolymer named (PVK) (Py) have been synthesized by oxidative coupling reaction and characterized by several physicochemical methods, then by a DFT chemical study we have shown through the study of the mechanism of copolymerization the existence of 4 intermediary oligomers (PP0, PP1, PP2 and PP3) [11]. These oligomers have been characterized and their electronic properties have been studied. To complete this study.

The objective is to suggest an oligomer model that reflect properties of the copolymer and test the possibility of proposing this oligomer or the corresponding copolymer for applications in the field of organic solar cells.



**Figure 1:** Structure of the studied copolymer PVK Py

### Computational methods

To calculate the unpaired electron spin densities of radical cations, we have used the density functional theory (DFT) of three-parameter compound functional of Becke (B3LYP) and the 6-31G (d, p) basis set for all calculations [12,13]. The geometric structures of neutral molecules were optimized within no constraints. Moreover, geometry structures of radical cations were optimized independently from the neutral molecules prior to the calculations of spin densities. The HOMO, LUMO and gap's energies were also deduced for the stable structure of the neutral and oxidized forms. Electronic transition energies and oscillator strengths of oligomers were obtained by TD/B3LYP method [14]. All calculations were executed employing the Gaussian 09 program [15].

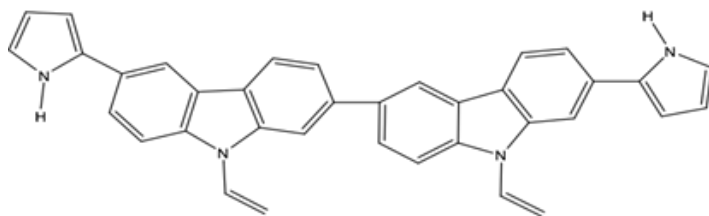
### Results and discussion

#### Mechanism

The PVKPy copolymer was prepared by our research group and characterized by modern spectroscopic methods [16]. Characterization by Diffraction X has shown that this copolymer is amorphous, so the internal architecture or the organization of the monomer units remains unknown whereas we have demonstrated in

previous works that there is a strong correlation between the structure, the organization of monomer units and electronic properties [17]. In this first part, we will propose a mechanism for polymerization of the two monomers PVK and Py using the spin density calculation technique. To do so, for each step, we will optimize the intermediary structures and we will determine for each structure the spin densities that will help us to propose the reactive sites and subsequently the polymerization mechanism. To facilitate calculations, we used N-vinylcarbazole instead of PVK. Let us remember that a principally accepted mechanism for the coupling reaction of conjugated monomers, which includes of two-step reactions. The first step is one-electron oxidation of the monomer to compose its radical cation. The second step is a coupling reaction of two radical cations to form a dihydro-dimer cation, which is followed by the expulsion of two protons to form a neutral dimer [18]. For exploring the initiating and propagating reactions, it is conceivable to admit that coupling reactions preferentially occurred between carbons having higher spin densities of carbazole firstly to form the dimer of carbazole (CbzCbz).

Then, when each pyrrole (Py) reacts with the end of this dimer, we can produce the oligomer named PCbzCbzP (Oligo 0) as shown in Figure 2.

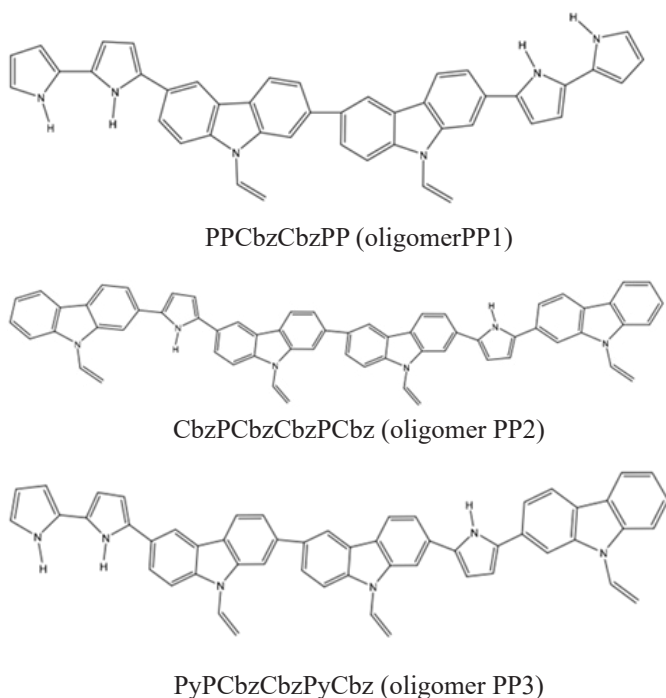


**Figure 2:** PCbzCbzP (oligomer PP0)

In the reaction medium, we have pyrrole and vinylcarbazole. The reaction could be continued according to three reaction schemes:

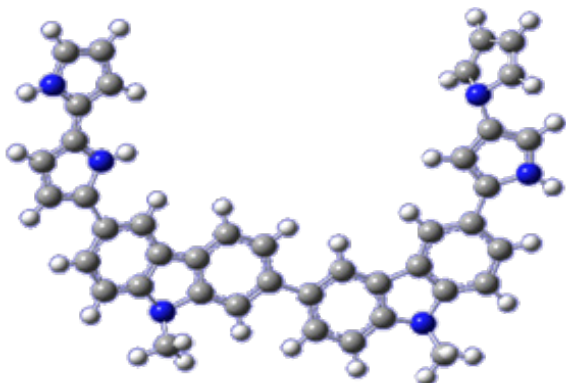
- Two pyrroles couple on both ends of oligomer 0 to form oligomer 1 (PPCbzCbzPP);
- Two vinyl carbazoles will couple on both ends to form oligomer 2 (CbzPCbzCbzPCbz);
- The pyrrole will react on one side and the carbazole will react on the other side to form the oligomer 3 (PPCbzCbzPCbz).

Figure 3 resume the reaction paths of succeeding coupling reaction of PCbzP founded on calculated spin densities. Three oligomers can be produced as we can show in Figure 3.



**Figure 3:** Studied oligomers (PP1, PP2 and PP3).

In accordance with the experimental preparation of the copolymer (PVKPy) *n*, we considered that firstly we formed a cross-linked PVK, then, when we added the pyrrole Py it oxidizes to constitute a radical cation. Considering the oxidation of dimer is easier than that of the monomer; the reactivity of the second step ought to be between a radical cation of this dimer (PVKPVK) and the radical cation of Pyrrole to shape PyPVKPVKPy, then the radical cation of Pyrrole or PVK. Regarding our theoretical study basis on calculated spin densities, we have suggested four oligomer structures. The first oligomer (oligo 1), shown in Figure 4, seems to be the better reflecting the experimental properties



**Figure 4:** Optimized structure of ppCbzCbzpp (oligomer 1) by B3LYP/6-31G (d) level

### Electronic Properties

Knowing that the energies of the HOMO and LUMO frontier

orbitals as well as the Gap energy play an important role if we want to propose these structures for photovoltaic applications, we have started by optimizing the proposed structures proposed by the mechanism (oligo *i* = 0, 1, 2 and 3) using the B3lyp/6-31G (d, p) method and from the most stable conformation of each oligomer, we have determined the values of the energies HOMO (the highest occupied molecular orbital), LUMO (lowest unoccupied molecular orbital) and of course the energy of the gap ( $\Delta E$ ) which corresponds to the difference between the preceding energies. In Table 1 we have collected the obtained results.

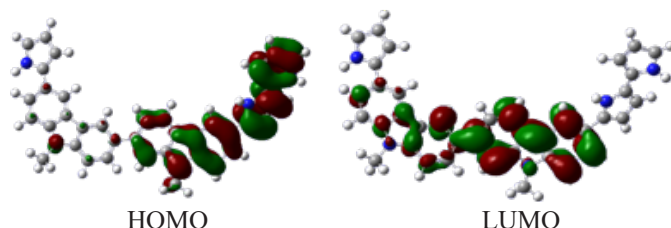
**Table 1:** Calculated HOMO (eV), LUMO (eV), Egap (eV) of the three oligomers obtained at DFT/B3LYP/6-31(d,p) level.

Compounds	EHOMO (eV)	ELUMO (eV)	$\Delta E(\text{gap})$ (eV)
Oligomer 0	-4.734	-0.848	3.88
Oligomer 1	-4.393	-0.849	3.54
Oligomer2	-4.418	-0.838	3.58
Oligomer 3	-4.433	-0.859	3.57

### The Analysis of the Results Revealed the Following Findings

The HOMO and LUMO energies are stabilized or destabilized according to the type of structure and the organization of the monomers Cbz, Py; in fact the HOMO energies are classified in the following order EHOMO (Oligomer 0) <EHOMO (Oligomer 3) <EHOMO (Oligomer 2) <EHOMO (Oligomer 1) whereas the LUMO energies are classified in the following order: ELUMO (Oligomer 3) <ELUMO (Oligomer 1) <ELUMO (Oligomer 0) <ELUMO (Oligomer 2). We find that HOMO orbitals are stabilized by the addition of monomers whatever their nature.

The order of energy gaps is Oligomer 1 (3, 54eV) <Oligomer 3 (3.57eV) <Oligomer 2 (3.58eV) <Oligomer 0 (3.88eV). This shows that oligomer 1 having an organized structure in the form of a block of two Cbz monomer followed by two Py monomers is the best in term of the conjugation properties since it possesses the weakest gap. In view of the obtained optimized geometries, we have presented in Figure 5 an example of the frontier orbital HOMO and LUMO of oligomer 1.

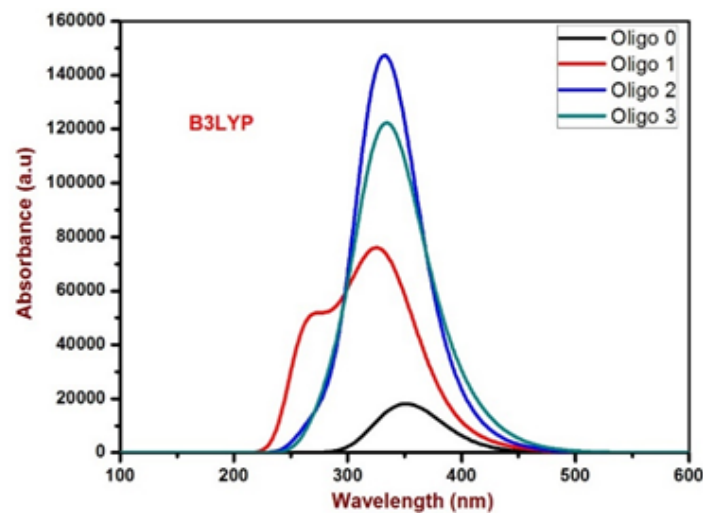


**Figure 5:** Obtained isodensity plots of the frontier orbital HOMO and LUMO of oligomer 1 (PPCbzCbzPP) obtained at DFT/B3LYP/6-31(d) level.

On the other hand, it is significant to examine the HOMO and the LUMO for these compounds because the relative ordering of occupied and virtual orbital affords a conceivable qualitative indication of excitation properties and the ability of electron hole transport. Generally, as plotted in figure 5, the HOMO owns an antibonding character between the consecutive subunits; whilst the LUMO of all compounds mostly shows a bonding character between the subunits.

### Optical Properties

From the optimized molecular structures obtained with B3LYP/6-31G (d,p) method, the UV-vis spectra of each studied compounds (oligomer 0, oligomer 1, oligomer 2 and oligomer 3) have been calculated using TD-DFT/B3LYP. The results obtained are presented in the form of Figure 6 and Table 2.



**Figure 6:** Simulated UV-visible optical absorption spectra of the studied compound obtained by the TD-DFT: B3LYP/6-31G (d,p) level.

The corresponding simulated UV-Vis absorption spectra of all studied oligomers are shown in Figure 6. We can get the values of the absorption maximum  $\lambda_{max}$  (nm) and oscillator strength (O.S) alongside with fundamental excitation configuration of the studied compounds. In addition, we have note that the broader absorption peak means that there is a distribution of energy level corresponding to the  $\pi-\pi^*$  transition. Excitation to the S1 state corresponds

exclusively to the promotion of an electron from the HOMO to the LUMO. The absorption wavelengths occurring from S0→S1 electronic transition raises progressively with the increasing of conjugation lengths. It is reasonable, as HOMO→LUMO transition is predominating in S0→S1 electronic transition; the results are a decrease of the LUMO and an increase of the HOMO energy.

**Table 2:** Transition states, assignments, the corresponding wavelength, and oscillator strength for the Oligomer 1 by TD-DFT// B3LYP/6-31G (d,p)

Compounds	$\lambda_{max}$ (nm)	Ea (eV)	O. S	Transition states
Oligomer 0	364.62	3.40	0.14	HOMO->LUMO (87%)
Oligomer 1	398.73	3.10	0.07	HOMO->LUMO (96%)
Oligomer 2	390.20	3.17	0.14	HOMO->LUMO (96%)
Oligomer 3	394.31	3.14	0.16	HOMO->LUMO (83%)

The calculated wavelength  $\lambda_{max}$  of the studied compounds (oligo0, oligo1, oligo2 and oligo3) decreases in the following order  $\lambda_{max}$  (oligomer 1)> $\lambda_{max}$  (oligomer 3)> $\lambda_{max}$  (oligomer 2)> $\lambda_{max}$  (oligomer 0), which is the same order of the reduction of the acceptor strength. This bathochromic effect from oligo 0 to oligomer 1 is evidently due to a higher mean conjugation length and to inter-chain electronic coupling [19]. We have noted at the same time that oligomer 1 has the best absorption properties (398.73 nm); this confirms the results obtained in the first part where we have showed that it is the oligomer that has the best properties of conjugation (Egap = 3.54 eV).

### Photovoltaic Properties

Concerning the study of Photovoltaic Properties and knowing that generally, the most efficient material solar cells are based on the bulk hetero-junction structure of the blend of  $\pi$ -conjugated molecule or polymer donors and fullerene derivative acceptors [20-22]. Here, we have studied and discussed the photovoltaic properties of the proposed compounds oligomer 0, oligomer 1, oligomer 2 and oligomer 3 as donor mixed with [6.6]-phenyl-C61-butyric acid methyl ester (PCBM), which is the most widely used as an acceptor in solar cell devices. The HOMO and the LUMO energy levels of the donor and acceptor components are very important



factors to determine whether effective charge transfer will happen between donor and acceptor. To evaluate the possibilities of electron transfer from the studied oligomers (Oligomer 0, 1, 2, and 3) to the conductive band of PCBM or derivatives, the HOMO and LUMO levels were compared.

On the other hand, and from the above analysis, we know that the LUMO energy levels of the studied molecules are much higher than that of the ITO conduction band edge (-4.7 eV). Thereby, the studied molecules oligomer 1, oligomer 2 and oligomer 3 have a strong ability to inject electrons into ITO electrodes (the HOMO energy of oligomer 0 is about -4.73 eV lower than that of the ITO conduction band edge (-4.7 eV), so we eliminated this oligomer). The experiment phenomenon is quite consistent with previous literature, this latter reported that the increase of the HOMO levels may suggest a negative effect on organic solar cell performance due to the broader gap between the HOMO level of the organic molecules and the HOMO level of several acceptor PCBM. (C78-C2V, C78-D3, C84-D2, C84-D2d) [22].

As shown in Table 3, both HOMO and LUMO levels of the studied molecules agree well with the exigency for an efficient photosensitizer. It should be noted that the LUMO levels of the studied com-

pounds are higher than that of PCBM derivatives, which varies in literature from -4.0 to -3.94 eV (C84-D2d (-3.95eV), C78-C2V (-3.94), C78-D3 (-4.0), C84-D2 (-3.98)) [22]. To evaluate the possibilities of electron transfer from the studied molecules to the conductive band of the proposed acceptors, the HOMO and LUMO levels are compared. Knowing that in organic solar cells, the open circuit voltage is found to be linearly dependent on the HOMO level of the donor and the LUMO level of the acceptor. The maximum open circuit voltage ( $V_{oc}$ ) of the BHJ solar cell is related to the difference between the highest occupied molecular orbital (HOMO) of the donor (our studied compounds) and the LUMO of the electron acceptor (PCBM derivatives in our case), taking into account the energy lost during the photo-charge generation [22,23]. We have calculated the theoretical values of open-circuit voltage  $V_{oc}$  from the following expression [24].

$$V_{oc} = \frac{1}{e} (|E_{HOMO}(\text{Donor})| - |E_{LUMO}(\text{Acceptor})| - 0.3)$$

Also,  $\alpha$  is determined by the difference between the LUMO energy levels of the studied compounds and the LUMO energy level of PCBM derivatives [25].

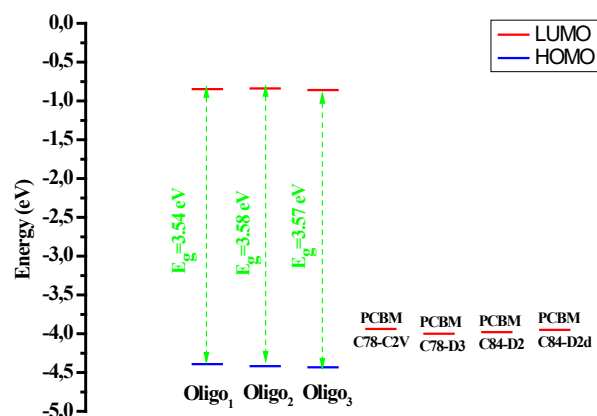
$$\alpha = E_{LUMO}(\text{Donor}) - E_{LUMO}(\text{Acceptor})$$

**Table 3: Energy values of ELUMO (eV), EHOMO (eV), Egap (eV) and the open circuit voltage Voc (eV) of oligomer 1, 2 and 3 obtained by B3LYP/6-31G(d)**

Compounds	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	PCBM C78-C2V	PCBM C78- D3	PCBM C84- D2	PCBM C84-D2d
			$V_{oc}$ (eV)	$V_{oc}$ (eV)	$V_{oc}$ (eV)	$V_{oc}$ (eV)
Oligomer 1	-4.393	-0.849	0.15	0.09	0.11	0.14
Oligomer 2	-4.418	-0.838	0.17	0.12	0.14	0.17
Oligomer 3	-4.433	-0.859	0.19	0.13	0.15	0.18
PCBMC78-C2V	-	-3.94	-	-	-	-
PCBM C78-D3	-	-4.00	-	-	-	-
PCBM C84-D2	-	-3.98	-	-	-	-
PCBM C84-D2d	-	-3.95	-	-	-	-

The acquiring values of  $V_{oc}$  of the 3 oligomers (oligomer 1, oligomer 2 and oligomer 3) range respectively from (0.153 eV; 0.178 eV; 0.193 eV) for PCBM C78-C2V; (0.093 eV; 0.118 eV; 0.133 eV) for PCBM C78-D3; (0.113 eV; 0.138 eV; 0.153 eV) for PCBM C84-D2 and (0.143 eV; 0.168 eV; 0.183 eV) for PCBM C84-D2d (see Table 3). These values are good enough for a possible electron injection.

Therefore, all our compounds can be used as BHJ because the electron injection process from the studied molecule to the conduction band of PCBM derivatives and the subsequent regeneration is possible in an organic solar cell. Figure 7 shows detailed data of energy of the frontier orbitals for studying compounds with PCBM and its derivatives.



**Figure 7: Sketch of DFT/B3LYP/6-31G (d) calculated energy of the HOMO, LUMO levels of the oligomer 1, 2 and 3**

## Conclusion

The results of this study show that:

- The reactivity for coupling reaction between pyrrole and poly-vinylcarbazole are deduced from the calculated unpaired electron spin densities of the respective radical cations.
- The major regioselective products of the polymerization reactions were well understood in term of the magnitude of calculated spin densities of several oligomers.
- We have predicted the most oligomerization mechanism via the proposed reaction paths of the succeeding coupling reactions of these two monomers. Four oligomers can be generated and according to the experimental results, it appears that the structure of the oligo 1 (PPCbzCbzPP) seems to be the better reflecting the experimental properties.
- The results of the optimized structures for all studied compounds showed that they have similar conformations (quasi planar conformation). We found that the modification of several groups does not change the geometric parameters.
- The calculated frontier orbital energies HOMO and LUMO and energy gaps showed that the energy  $E_{gap}$  of the studied molecules differ slightly from 3.886 eV to 3.544 eV depending on the different structures. Also, we can remark that the energy  $E_{gap}$  decreases in this following order: Oligomer 1 (3.54 eV) < Oligomer 3 (3.57 eV) < Oligomer 2 (3.58 eV) < Oligomer 0 (3.88 eV). This is presumably due to the effect of the conjugated system in the studied compounds.
- The compound oligomer 1 (PyPyPVKPVKPyPy) have a relatively high value of  $\lambda_{max}$  (398,73nm) and the smaller gap energy (3,544 eV) is expected to have the most outstanding photo physical properties.
- To see the possibility to suggest these materials for organic solar cell application,
- photovoltaic properties were determined by taking acceptors 4 derived from PCBM,
- only the molecules oligomer 1, oligomer 2 and oligomer 3 can be proposed as sensitizers because the electron injection process to the conduction band of the acceptor (PCBM and derivatives) and the subsequent regeneration is possible.
- This calculation procedure can be used as a model system for understanding the relationships between electronic properties and molecular structure and can be utilized to explore their suitability in electroluminescent devices and in related applications. Probably, the procedures of theoretical calculations can be employed to predict and undertake the electronic properties on yet prepared and efficiency proved other materials.

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