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Design and TDDFT Study of The Novel Structures Similar to BODIPY with Prominent Fluorescence Properties

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ABSTRACT

Functional dye is a new term in the field of dye chemistry which has been specifically designed for high-technology applications such as solar cells, photochromic dyes, liquid crystal, electrophotography, fluorescent sensors and photodynamic therapy. BODIPY and its derivatives as organic fluorophores have optical properties and can be used as potential sensors in various applications for biotechnological, industrial and medical purposes. In this research, a group of a new fluorescent indicators based on BODIPY structure were designed which have been composed from two seven-membered rings including Al or B atoms that has been connected with methine bridge complexed with NH_2 or PH_2 center. The geometries, optical properties and electronic structures of various designed molecules were studied using time-dependent density functional theory (TDDFT). The results of the calculations showed that the new designed structures are stable and highly optically active with considerable quantum yield (Φ) absorption and emission as if is promising candidates for hi-tech different applications.

Keywords: BODIPY; Computational; Conjugated System**;** Fluorescence; Functional dyes; Optical Properties; TDDFT

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Introduction

Functional dyes have low optical band gaps energy and also near-infrared (NIR) absorbing and emitting properties. These fluorescent dyes have attracted tremendous attention and investigated intensively in recent years due to their practical uses in various noteworthy arenas such as imaging and sensing in bio-systems [1], photo dynamic therapy [2-3], optical recording [4], and organic photovoltaic solar cells [5]. Light in the near-infrared (NIR) zone has the benefits of deeper penetration as the results of lower absorption and scattering of light [6]. Therefore, various efforts were done to design and synthesis of the dyes with favorable and attractive properties, for instance, the NIR dyes based on cyanines [7-8], porphyrins and phthalocyanines [9-11], rhodamines [12] and other dyes [13-15] were proposed. The boron-dipyrromethenes (BODIPYs), a class of organic fluorophores [16-17] are unique dyes which have a versatile and tunable optical properties, small Stokes shift, relatively chemically inert, high solubility in many organic solvents[18-19]. They have excellent stability and intense UV absorption followed by sharp fluorescence emission with high quantum yields which make the BODIPY suitable for utilizing as a fluorescent indicator [20], probe for the fluorescence imaging of biomolecules in living systems [21], dye in photodynamic therapy [22-23], fluorescent pH probes [24], photo-induced electron transfer [25], dye with NLO properties [26], light-harvesting antenna [27], multiple logic operations for the detection of CO2 gas [28] and appropriate in monitoring of polymerization process [29]. Various efforts were done to adjust and tune the optical properties of BODIPY [30-34]. Polarity, dielectric constant and refractive index of solvents play an important role on structure, stability, electronic and spectroscopic properties and reactivity of different chemical systems [35-37]. Many quantum chemical computations studies were performed for investigation of solvent effect on optical and electrical properties of rhenabenzyne complex [38], Ru(PH3)4(η2-benzyne) complex [36], Ni(CO)2(NHC)2 complex (NHC = 1H-imidazol-2-ylidene) [39], (OC)4Cr-biscarbene complex [40]. Absorption and emission spectra of three BODIPY dyes were calculated for few solvents by DFT and TDDFT methods [41]. The solvent polarity effect from hexane to DMSO were obtained using computational method for a number of BODIPY dyes in the ground and excited states using DFT and TDDFT methods, respectively [42]. The Excited states study are extremely important for

several areas such as fluorescence, photochemistry, photodynamic therapy and photocatalysis [43]. TDDFT methods are generally used for computational investigation of structure and electrical properties of molecules in excited states. The molecular behaviors and electronic properties of (CO)4Crbiscarbene and osmabenzyne complex were studied using computational methods in ground states and excited state [40,44]. In this research, the BODIPY molecule was considered as a reference molecule to design new molecules with better and more optimal electrical and optical properties.

Computational Details

BODIPY dyes contain a conjugated system of two pyrrole rings connected by methine group and complexed by the difluoroboron moiety, typically BF_2. In this research, similar to BODIPY, three structures were designed which were shown in Fig. 1.

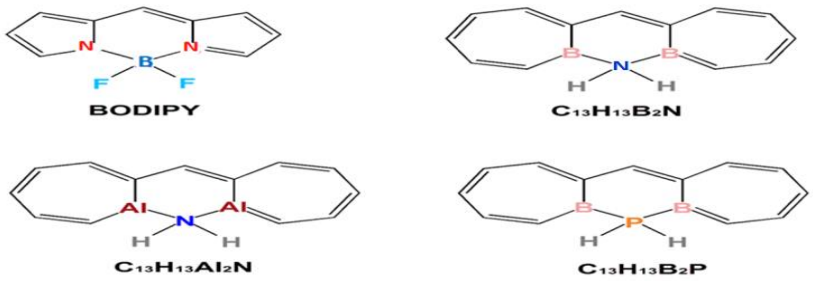


Fig. 1. The structure of BODIPY and three designed molecules similar to it.

In designing the molecules two five member rings of BODIPY molecule were changed with seven member rings, also the nitrogen atoms in it were replaced by boron or aluminium atoms to obey the Hückel's rule for aromaticity (4n+2 delocalized π-electrons). Finally, the BF_2 group was replaced by NH_2 or PH_2 groups. All structures were optimized using M062X [45] and ωB97XD [46-47] correlation functional methods and 6-311G(d,p) and 6-311++G(d,p) basis sets[48-49]. The M06-2X method is well suited for a broad range of applications on main-group chemistry, transition-metal chemistry, and molecular structure prediction which has a high nonlocality

functional with double the amount of nonlocal exchange (2X). The ωB97XD is a long-range corrected hybrid density functional with damped atom–atom dispersion corrections and has been found more reliable for the calculation of the dispersion as well as charge transfer (CT) excited states than results found using earlier density functional [41,42].

Vibrational frequencies were implemented at the same level of theory to confirm all structures are in global minimal. All calculations were carried out using Gaussian 09 package [48]. The electronic density of state for all optimized structures calculations were done using GaussSum 03 [49]. Gap energy (E_g) was calculated based on DOS results using the following expression:

$$\mathbf{E_g = E_{LUMO} - E_{HOMO}}$$

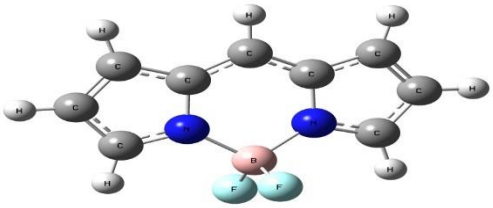
Where, E_{HOMO} refer to the energy of highest occupied molecular orbital (HOMO) and E_{LUMO} refer to the energy of lowest unoccupied molecular orbital (LUMO). For all structures, the UV-visible absorption spectra of these compounds were calculated using time-dependent density functional theory (TDDFT) employing the B3LYP, ωB97XD, M062X method and 6-311G(d,p) basis set [50-53]. Two simultaneous methods were used to confirm the obtained data. The solvent effect on optical properties was calculated in TDDFT in ωB97XD/6-311G(d,p) computational level and CPCM model [54]. The conductor-like PCM (C-PCM) in which the continuum is conductor-like similar to COSMO solvation model, a calculation method for determining the electrostatic interaction of a molecule with a solvent, is commonly used in computational chemistry to model solvation effects. The SCRF (Self-Consistent Reaction Field) model which was used in the solvent effect calculations is a method of accounting for the effect of a polarizable solvent (and optionally, a classical macromolecular system) on the quantum system [35,38,40].

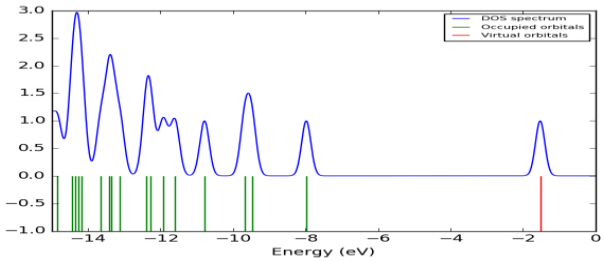
Results and Discussion

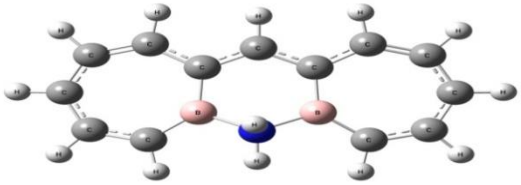
Optimized Structures

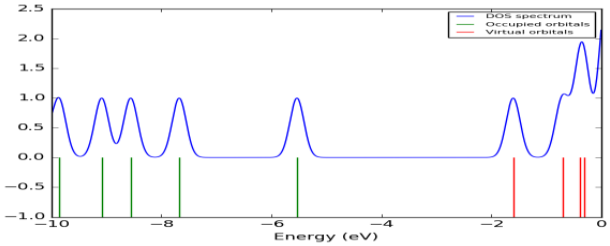
The structure of BODIPY molecule and three designed structures were optimized using M062X and ωB97XD methods and 6-311G(d,p) and 6-311++G(d,p) basis sets. The optimized structures

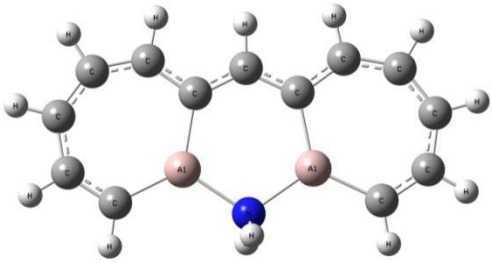
of BODIPY and three other structures performance using M062X/6-311++G(d,p) were shown in Fig. 2.

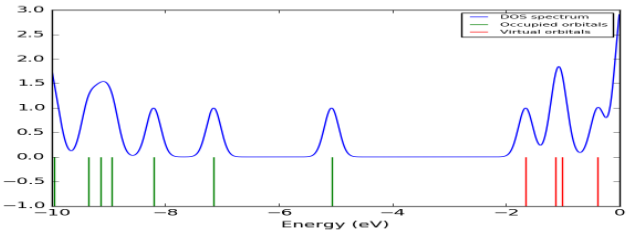












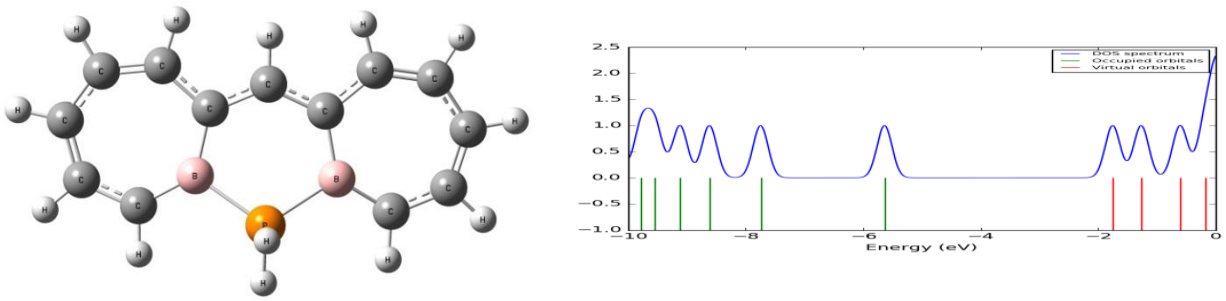


Fig. 2. Optimized structures of BODIPY and three designed structures.

For all optimized structures the frequency analysis was performed to show that all the structures are in global minimal. In table 1, the results of calculated first frequency for these molecules were reported.

Table 1. The results of calculated first frequency for designed molecules.

Molecule	ωB97XD /6-311G(d,p)	ωB97XD /6-311++G(d,p)	M062X/6-311G(d,p)	M062X/6-311++G(d,p)
BODIPY	6.4	12.1	10.2	22.7
$C_{13}H_{13}B_2N$	45.2	45.0	44.9	44.6
$C_{13}H_{13}Al_2N$	13.6	2.8	13.0	27.5
$C_{13}H_{13}B_2P$	36.8	36.8	38.2	37.4

As presented in table 1, frequency calculations show that the all structures for each methods and basis sets must be stable and in local minima. In continue, the dihedral angle between the carbon atoms in three side and nitrogen (or phosphorus) in one place was analyzed to estimate the flatness of molecules. The dihedral angles for each molecule calculated by four different methods, which were presented in table 2.

Table 2. The dihedral angles for each molecule calculated by four different methods.

Molecule	ωB97XD /6-311G(d,p)	ωB97XD /6-311++G(d,p)	M062X/6-311G(d,p)	M062X/6-311++G(d,p)
BODIPY	0	0	0	0
C13H13B2N	40.4	40.1	40.5	40.1
C13H13Al2N	0.14	0.13	9.5	17.9
C13H13B2P	44.8	45.0	44.9	45.0

Electrical properties

Since exhibition of electrical properties it is very important for various applications in the academic and industrial area, the electrical properties of proposed molecules were studied using the orbitals density of states.

Table 3. The values of E_{HOMO}, E_{LUMO} and E_g for the BODIPY, and the designed molecules

Molecule	E_{HOMO}		E_{LUMO}		E_g	
	M062X/6-311G(d,p)	M062X/6-311++G(d,p)	M062X/6-311G(d,p)	M062X/6-311++G(d,p)	M062X/6-311G(d,p)	M062X/6-311++G(d,p)
BODIPY	-7.33	-7.42	-2.41	-2.54	4.92	4.88
$C_{13}H_{13}B_2N$	-5.45	-5.53	-1.46	-1.6	3.99	3.93
$C_{13}H_{13}Al_2N$	-4.96	-5.07	-1.5	-1.65	3.46	3.42
$C_{13}H_{13}B_2P$	-5.57	-5.63	-1.63	-1.75	3.94	3.88

As illustrated in table3, the designed molecules have lower E_g which is consequence of higher degree of conjugation in them.

Optical Properties

The optical properties of BODIPY and designed structures, using TDDFT methods with different functionals, were calculated. In table 4-6, the calculated UV-visible absorption for BODIPY and offered molecules has been compared calculated by B3LYP, ωB97XD and M062X method respectively.

Table 4. Calculated UV-visible absorption for BODIPY and designed molecules using TD-B3LYP.

Molecule	BODIPY		$C_{13}H_{13}B_2N$		$C_{13}H_{13}Al_2N$		$C_{13}H_{13}B_2P$	
	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*
1	394.13	0.3714	511.51	0.4113	603.77	0.0193	591.20	0.0179
2	339.50	0.2255	483.82	0.0179	595.77	0.4652	530.81	0.3615
3	329.04	0.0267	426.57	0.1984	545.70	0.0093	454.40	0.1303
4					462.01	0.1944		

Table 5. Calculated UV-visible absorption for BODIPY and designed molecules using TD-ωB97XD.

Molecule	BODIPY		$C_{13}H_{13}B_2N$		$C_{13}H_{13}Al_2N$		$C_{13}H_{13}B_2P$	
	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*
1	391.90	0.5437	522.33	0.5110	616.17	0.5711	543.26	0.4558
2	308.90	0.1199	426.84	0.0307	525.02	0.0322	514.41	0.0281
3	292.48	0.0393	380.64	0.1953	422.47	0.0154	400.83	0.1755
4					410.28	0.2374		

Table 6. Calculated UV-visible absorption for BODIPY and designed molecules using TD-M062X.

Molecule	BODIPY		$C_{13}H_{13}B_2N$		$C_{13}H_{13}Al_2N$		$C_{13}H_{13}B_2P$	
	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*
1	399.69	0.5012	525.68	0.4733	616.86	0.5314	546.39	0.4162
2	303.22	0.1281	439.12	0.0286	556.84	0.0273	527.58	0.0261
3	288.41	0.0409	388.54	0.2097	466.83	0.0122	411.36	0.1782
4					425.65	0.2280		

In tables 4-6 obviously it has been demonstrated that, in comparison to BODIPY, the notable modification in optical properties was done in designed molecules. In BODIPY only has one

absorption band near the visible region of light however the designed molecules have absorption lines in visible region. Between the designed molecules, the $C_{13}H_{13}Al_2N$ molecule has better improvement in optical properties which may be the result of higher degree of its planar shape in comparison to others.

Emission spectrum

BODIPY dyes are noteworthy for sharp excitation and emission peaks contributing to brightness. The absorption and emission spectral data of BODIPY molecule and three designed structures are shown in in the following table and figures.

Table 7. The calculated emission data for BODIPY and designed molecules.

Molecule	BODIPY		$C_{13}H_{13}B_2N$		$C_{13}H_{13}Al_2N$		$C_{13}H_{13}B_2P$	
	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*
1	412.03	0.4235	545.80	0.4928	636.36	0.5803	572.34	0.4282
2	311.38	0.1696	435.02	0.0287	538.25	0.0282	535.69	0.0250
3	294.44	0.0425	391.76	0.2199	472.00	0.0198	412.12	0.2079
4					415.01	0.2273		

In table 7, the emmision data for BODIPY and three designed molecules was reported. As obviously seen, the designed molecules have good flourescence emmision in larger wavelenght in comparison to BODIPY. In Fig 3-6, the absorption and emision spectra of BODIPY, $C_{13}H_{13}B_2N$, $C_{13}H_{13}Al_2N$ and $C_{13}H_{13}B_2P$ molecules were reported respectively.

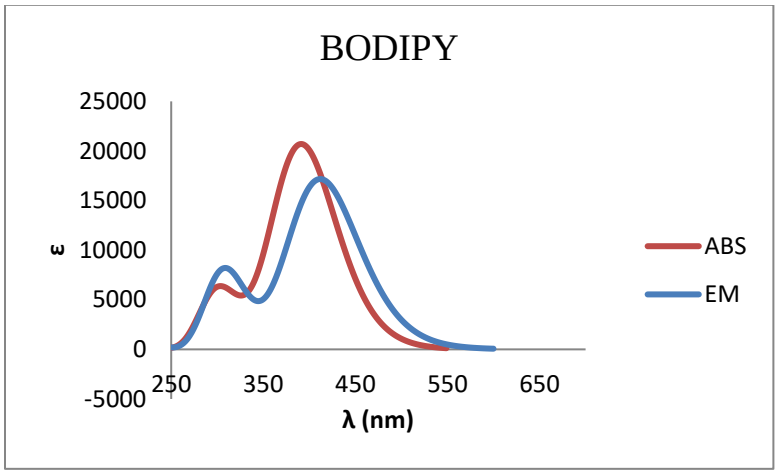


Fig. 3. The absorption and emission spectra for BODIPY molecule.

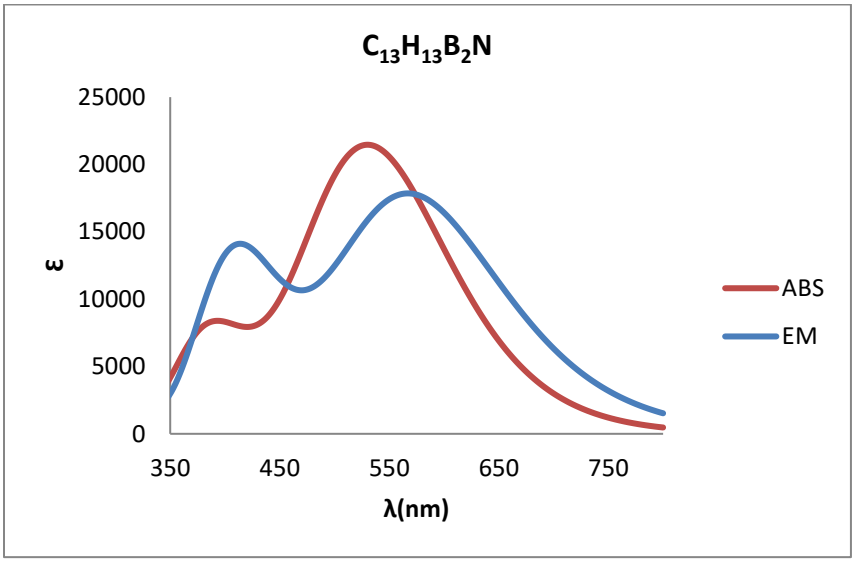


Fig. 4. The absorption and emission spectra for $C_{13}H_{13}B_2N$ molecule.

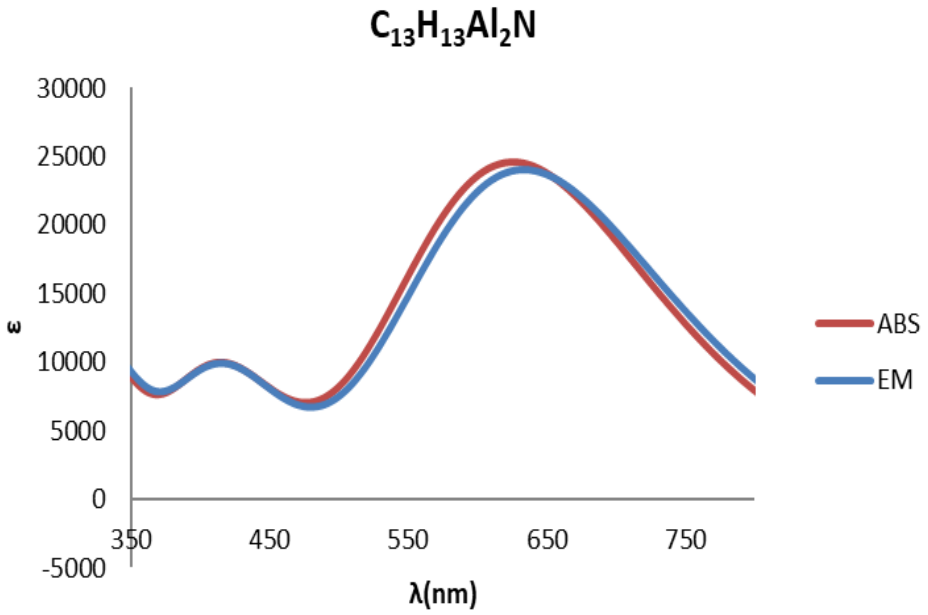


Fig. 5. The absorption and emission spectra for $C_{13}H_{13}Al_2N$ molecule

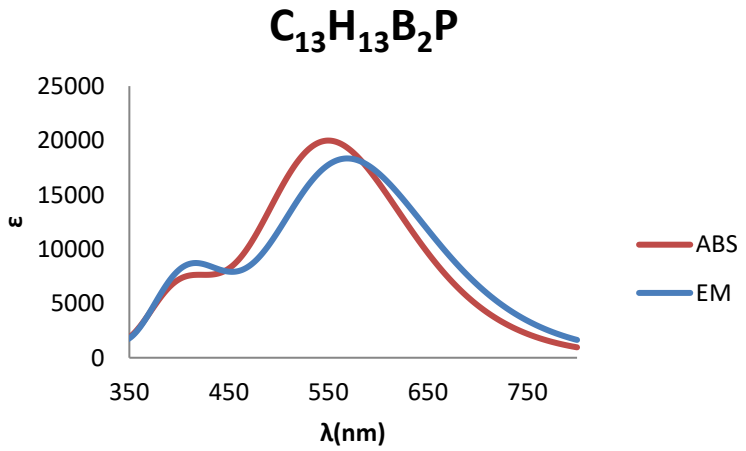


Fig. 6. The absorption and emission spectra for $C_{13}H_{13}B_2P$ molecule.

As depicted in Fig4-6, the designed molecules have intense absorption and emission in visible region with high quantum yield (Φ) which is a measure of the efficiency of photon emission.

Additionally, it was shown that between them the $C_{13}H_{13}Al_2N$ molecule has better optical properties and higher quantum yield and so is brighter fluorophore. In Fig 6 and 7 the absorption and emission of light by the BODIPY and $C_{13}H_{13}B_2N$ molecule are compared respectively.

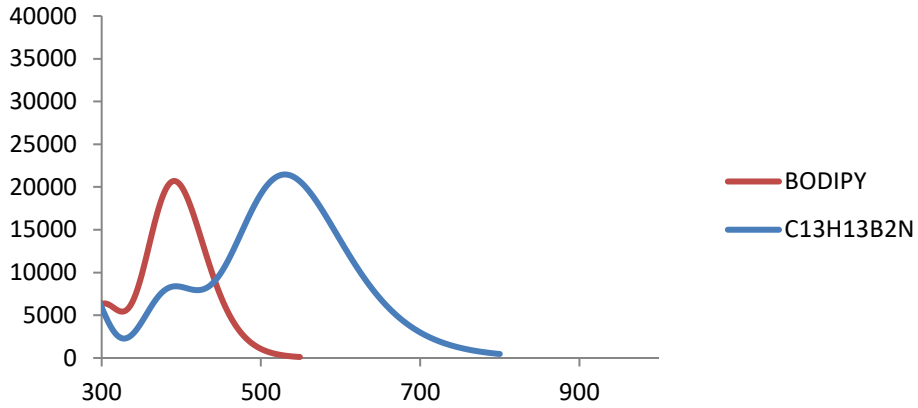


Fig. 7. The comparison of absorption spectra of BODIPY and $C_{13}H_{13}B_2N$ molecule

In Fig. 7 it was illustrated that, in comparison to the BODIPY, the $C_{13}H_{13}B_2N$ has more intense absorption in higher wavelength.

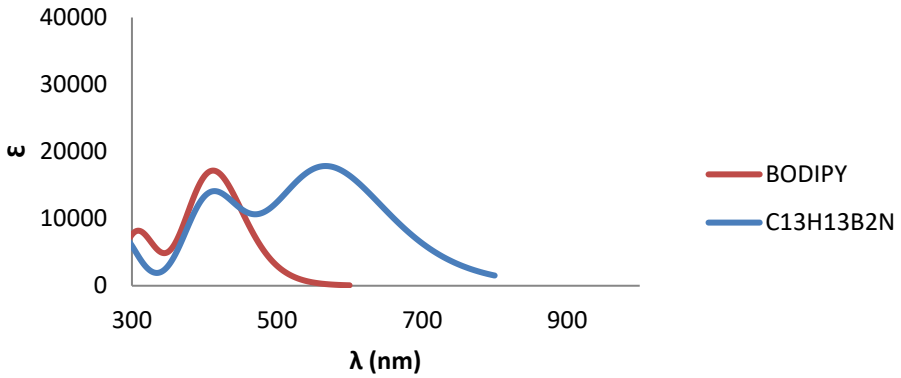


Fig. 8. The comparison of emission spectra of BODIPY and $C_{13}H_{13}B_2N$ molecule

Fig. 8 also shows that the $C_{13}H_{13}B_2N$ has more intense emission in wavelength about 550 nm which is larger than the 412 nm for BODIPY. As illustrated in Fig 7 and 8, compared to BODIPY,

the $C_{13}H_{13}B_2N$ has superior optical properties which have more intense absorption and emission in larger wavelength.

Solvent effects

For deducing the effect of solvents on optical properties, the TDDFT calculations in various solvents with different dielectric constants, using ωB97XD computational level at single point, were done. In tables 8-10, the UV-visible absorption for the designed molecules in H_2O, DMSO, CH_2Cl_2, CH_3Cl and acetone as solvents is reported.

Table 8. The UV-visible absorption for $C_{13}H_{13}B_2N$ in different solvents.

Solvent	Water		DMSO		Dichloromethane		Acetone		Chloroform	
	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*
1	555.74	0.6629	562.60	0.6889	563.61	0.6909	558.08	0.6712	565.70	0.6969
2	427.16	0.0463	427.98	0.0492	428.43	0.0494	427.56	0.0472	429.04	0.0500
3	383.32	0.2091	384.23	0.2103	384.57	0.2097	383.71	0.2092	385.07	0.2092

Table 9. The UV-visible absorption for $C_{13}H_{13}Al_2N$ in different solvents.

Solvent	Water		DMSO		Dichloromethane		Acetone		Chloroform	
	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*
1	653.08	0.7859	664.50	0.8100	668.38	0.8045	657.78	0.7908	674.14	0.8024
2	461.54	0.0666	463.35	0.0708	470.76	0.0682	464.81	0.0668	478.95	0.0663
3	388.22	0.2354	389.68	0.2395	393.22	0.2429	389.97	0.2379	397.13	0.2469

Table 10. The UV-visible absorption for $C_{13}H_{13}B_2P$ in different solvents.

Solvent	Water		DMSO		Dichloromethane		Acetone		Chloroform	
	λ(nm)	*f*	λ(nm)	Ƒ	λ(nm)	*f*	λ(nm)	*f*	λ(nm)	*f*

1	574.53	0.6289	581.26	0.6578	582.27	0.6591	576.83	0.6377	584.34	0.6647
2	503.33	0.0420	504.61	0.0444	506.55	0.0444	504.42	0.0427	508.80	0.0448
3	403.37	0.1943	404.32	0.1963	404.74	0.1960	403.80	0.1948	405.31	0.1961

Reported data in tables 8-10, demonstrates that the optical properties of these designed molecules depend on solvent nature and with increasing the solvent polarity, the absorption of light for these molecules have been blue-shifted.

Conclusions

In this research new fluorophores having structure similar to the BODIPY molecule were proposed. These near-infrared fluorochromes have $C_{13}H_{13}B_2N$, $C_{13}H_{13}Al_2N$ and $C_{13}H_{13}B_2P$ structural formula. In this study it was illustrated that the designed structures are stable which their stabilities confirmed by different computational level of theory. It was observed that the value of E_g for the designed molecules is lower than the BODIPY molecule which is considerable. It was shown that the suggested molecules are highly optically active which have intense absorption and emission in visible region and therefore they are good fluorophores. Between them the $C_{13}H_{13}Al_2N$ have higher optical activity with stronger absorption and emission (considerable Φ as quantum yield) in its spectrum. The solvent effects on optical properties were calculated and it was shown that by increasing the solvent polarity, the absorption of light for these molecules have been blue-shifted. This property shows that new designed molecules are promising candidates for various applications such as imaging and labeling.

Conflict of Interest:

The authors declare that they have no conflict of interest.

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