

Synthesis and Characterization of Potential Efficient Electroluminescent Materials: 2-Phenyl-5-[4-(4-phenylamino-2*H*-1,2,3-triazol-2-yl)]phenyl-1,3,4-oxadiazole Derivatives

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Recently, 1,3,4-oxadiazole-based on heterocyclic compounds were investigated as electroluminescent materials. In this work, we first introduce 1,2,3-triazole to synthesize a series of 1,3,4-oxadiazole–1,2,3-triazole hybrids derivatives as potential electroluminescent materials and explore the effect of modification of the 1,2,3-triazole moiety. The λ_{max} values of the UV–vis of 1,3,4-oxadiazole–1,2,3-triazole hybrids are promoted to longer wavelengths (340–350 nm) than the traditional 1,2,3-triazole derivatives (280–330 nm) in solutions and have a bathochromic shift to 350–360 nm in THF solution. The λ_{max} values of the photoluminescence (PL) spectra are in the range 406–480 nm in solutions. Compound **7h** evaporated to form films on quartz substrates, had a maximum at 455 nm and showed a red-shift ($\approx$40 nm) with respect to the solution spectrum. The solution fluorescence quantum yields (Φ_f) were measured, all of which fell into the range 0.65–0.76, and were determined relative to that of 2-phenyl-5-(4-biphenyl)-1,3,4-oxadiazole in benzene ($\Phi_f = 0.80$). 1,3,4-Oxadiazole–1,2,3-triazole hybrids derivatives show unclearly reversible reduction processes in cyclic voltammogram measurements. Following spectroscopic studies and observation of the electrochemical behaviors, 1,3,4-oxadiazole–1,2,3-triazole derivatives were determined to be highly potential efficient blue electroluminescent materials.

1,3,4-Oxadiazole derivatives have been widely exploited as electron-transporting, hole-blocking (ETHB) materials in electroluminescent (EL) devices due to their electron-deficient nature, their high thermal stability and high photoluminescence quantum yield (PLQL).[1,2] 1,3,4-Oxadiazole-based heterocyclic compounds have also been eagerly investigated, for example, 1,3,4-oxadiazole–pyridine hybrids,[3] 1,3,4-oxadiazole–pyrimidine hybrids,[4] 1,3,4-oxadiazole–carbazole,[5] and 1,3,4-oxadiazole–spirobifluorene.[6] Since the heterocyclic moieties on the molecular structure can provide improved hole injection, transport properties, and confer rigidity, we have developed and prepared three types of heteroaromatics electroluminescent materials: 1,3,4-oxadiazole–triazolopyridinone, 1,3,4-oxadiazole–pyrazole, and 1,3,4-oxadiazole–pyridine–carbazole derivatives.[7] In our previous investigations, most heterocyclic moieties (pyrazole, pyridine, and triazolopyridinone) on a 1,2,3-triazole core exhibited significant a bathochromic shift (red shift) due to the substitution effect of the conjugation system.

1,2,3-Triazole derivatives possess a multitude of biological and medicational activities.[8] In this paper, we first introduce 1,2,3-triazole to synthesize 1,3,4-oxadiazole–1,2,3-triazole hybrid derivatives as potential electroluminescent materials, and then explore the effect of modification of the 1,2,3-triazole moiety. Following spectroscopic studies and measurements of cyclic voltammogram measurements, 1,3,4-oxadiazole–1,2,3-triazole derivatives were determined to be potential highly efficient blue electroluminescent materials.

Results and Discussion

Synthesis of 1,3,4-Oxadiazole–1,2,3-Triazole Derivatives 7a–7h. New potential efficient blue electroluminescent materials of 1,3,4-oxadiazole–1,2,3-triazole hybrid derivatives **7a**–**7h** were synthesized and their synthetic routes are shown in Scheme 1. Sydnones have attracted extensive interest for biological, pharmaceutical, and synthetic applications and for their photochromic properties.[9,10] We have enthusiastically explored new applications of sydnones in electroluminescent materials by forming the 1,3,4-oxadiazole hybrid derivatives. The sydnone compounds **1** were easily converted to the 3-aryl-4-formylsydnone derivatives **2** in a solution of $POCl_3$ and DMF by the Schmidt reaction in 52–66% yields.[11] Following the literature procedure,[12] 3-(4-ethoxycarbonylbenzo)sydnone was dissolved in solution of EtOAc with a small amount of HClaq and stirred at room temperature to provide ethyl 4-hydrazinylbenzoate.

The 3-aryl-4-formylsydnone derivatives **2** were mixed with ethyl 4-hydrazinylbenzoate and stirred in an EtOH solution to achieve the elimination and give the corresponding products in good yields (**3a**–**3d**, 80–83%). The acidic decomposition of compounds **3a**–**3d** was performed in the acidic EtOAc solution; the sydnone rings rearranged and sequentially underwent ring opening and decarboxylation to provide the 4-arylamino-1,2,3-triazoles **4a**–**4d**.[10] Treating the 4-arylamino-1,2,3-triazoles **4a**–**4d** with hydrazine monohydrate according to the

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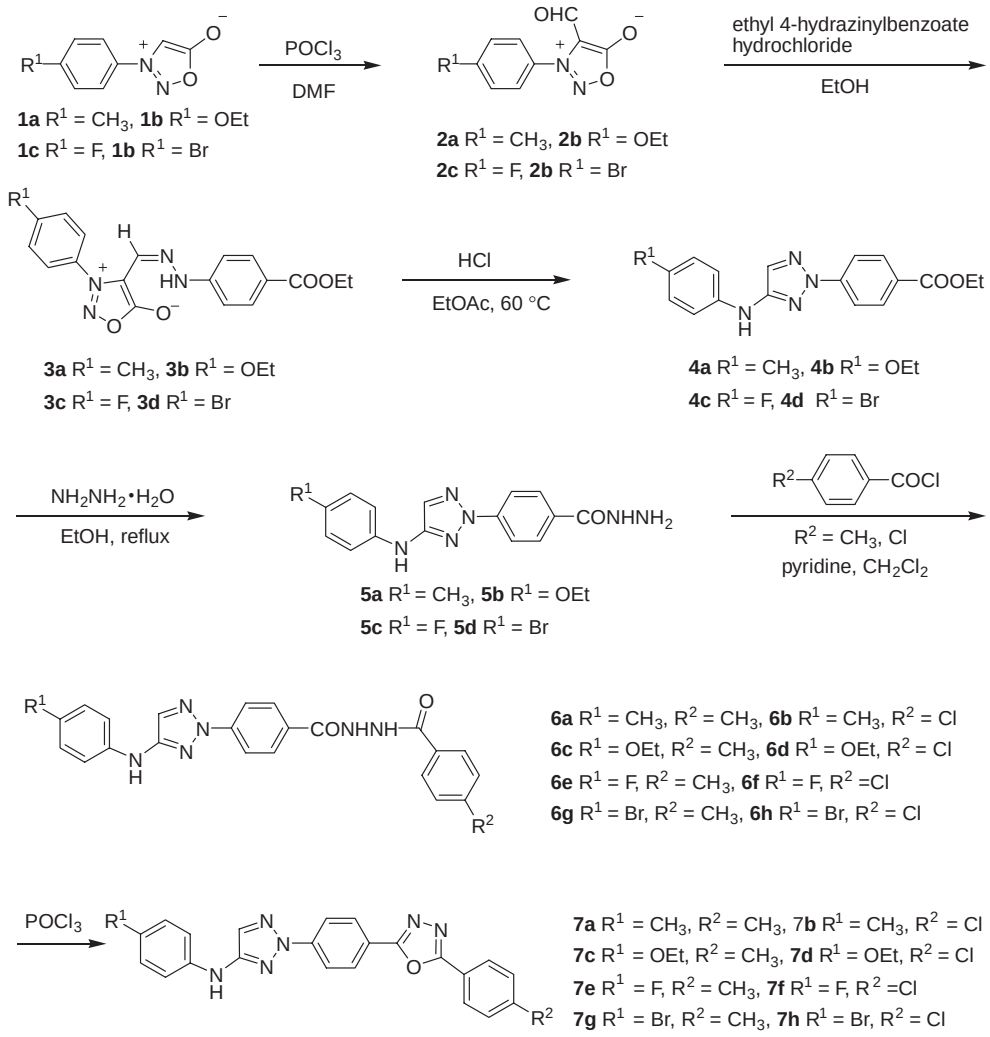

1a $R^1 = CH_3$, **1b** $R^1 = OEt$
1c $R^1 = F$, **1b** $R^1 = Br$

2a $R^1 = CH_3$, **2b** $R^1 = OEt$
2c $R^1 = F$, **2b** $R^1 = Br$

3a $R^1 = CH_3$, **3b** $R^1 = OEt$
3c $R^1 = F$, **3d** $R^1 = Br$

4a $R^1 = CH_3$, **4b** $R^1 = OEt$
4c $R^1 = F$, **4d** $R^1 = Br$

5a $R^1 = CH_3$, **5b** $R^1 = OEt$
5c $R^1 = F$, **5d** $R^1 = Br$

6a $R^1 = CH_3$, $R^2 = CH_3$, **6b** $R^1 = CH_3$, $R^2 = Cl$
6c $R^1 = OEt$, $R^2 = CH_3$, **6d** $R^1 = OEt$, $R^2 = Cl$
6e $R^1 = F$, $R^2 = CH_3$, **6f** $R^1 = F$, $R^2 = Cl$
6g $R^1 = Br$, $R^2 = CH_3$, **6h** $R^1 = Br$, $R^2 = Cl$

7a $R^1 = CH_3$, $R^2 = CH_3$, **7b** $R^1 = CH_3$, $R^2 = Cl$
7c $R^1 = OEt$, $R^2 = CH_3$, **7d** $R^1 = OEt$, $R^2 = Cl$
7e $R^1 = F$, $R^2 = CH_3$, **7f** $R^1 = F$, $R^2 = Cl$
7g $R^1 = Br$, $R^2 = CH_3$, **7h** $R^1 = Br$, $R^2 = Cl$

Scheme 1.

published reports[13] afforded benzohydrazide compounds **5a**–**5d** in 76–83% yields. Condensation of benzohydrazide compounds with benzoyl chloride yielded the bis(benzohydrazide) **6a**–**6h**. We treated the raw materials **6a**–**6h** directly with $POCl_3$[14] to obtain the cyclized 1,3,4-oxadiazole–1,2,3-triazole hybrid derivatives **7a**–**7h**, which could be purified easily by column chromatography. Their structures were determined by high-field NMR spectroscopy and CHN analysis.

Photophysical Properties. The UV–vis spectra of the 1,3,4-oxadiazole–1,2,3-triazole derivatives **7a**–**7h** were measured in THF, CH_2Cl_2, and $CHCl_3$ solutions. The λ_{max} values of **7a**–**7h** are in the range 340–350 nm in CH_2Cl_2 and $CHCl_3$ solutions and have a bathochromic shift to 350–360 nm in THF solution (see Table 1). The main absorptions of the low energy (π–π^*) transitions of the traditional 1,2,3-triazole derivatives are at 280–330 nm.[15] The 1,3,4-oxadiazole–1,2,3-triazole derivatives **7a**–**7h** exhibited significant red shifts due to the substitution effect of conjugation with the 1,3,4-oxadiazole moiety.[16] The long range of the substitution effects on R^1 and R^2 positions are not clearly a function of absorption and the results are shown in Table 1. The λ_{max} values of **7b** and **7d** are approximately at 354–358 nm in THF solution when the R^1-substituted group is CH_3 or OEt and R^2 is Cl group (see Fig. 1). The solution fluorescence quantum yields (Φ_f) of **7a**–**7h**, all of which fall in the range 0.65–0.76, were determined relative to that of 2-phenyl-5-(4-biphenyl)-1,3,4-oxadiazole in benzene ($\Phi_f = 0.80$).[17]

The photoluminescence (PL) spectra of 1,3,4-oxadiazole–1,2,3-triazole derivatives shown in Table 1 have λ_{max} values in the range 406–480 nm in CH_2Cl_2, $CHCl_3$, and THF solutions. Similar bathochromic shifts of the solvent effect (≈20 nm) are also found in the emission spectra in CH_2Cl_2 and THF solutions. The substitution effect of 1,2,3-triazole on the main core is a clear red-shift (≈30–100 nm) with respect to 2-*tert*-butylphenyl-5-biphenyl-1,3,4-oxadiazole (PBD, 370 nm).[15] The compounds of **7c** and **7d**, including the electron-donating group (R^1 = OEt), exhibit an intense deep-blue fluorescence in CH_2Cl_2 and THF solutions (λ_{max}s of PL is 470–480 nm, Table 1 and Fig. 2). The PL spectrum of **7h** of vacuum evaporated films on quartz substrates, with a maximum at 455 nm, shows a red-shift (≈40 nm) with respect to the solution spectrum, as shown in Fig. 3.

Cyclic Voltammetry Measurements. The electrochemical behaviors of the 1,3,4-oxadiazole–1,2,3-triazole derivatives **7a**–**7h** were investigated by cyclic voltammetry in solution. The measurements were carried out at a platinum electrode

Table 1. UV–Vis Absorption Maxima and Photoluminescence Peak Wavelength of 1,3,4-Oxadiazole–1,2,3-Triazole Derivatives **7a–7h**

	Compound		λ_{max}/nm of UV–vis			λ_{max}/nm of PL			Φ_f[a]
	R^1	R^2	$CHCl_3$	CH_2Cl_2	THF	$CHCl_3$	CH_2Cl_2	THF	
7a	$-CH_3$	$-CH_3$	348	348	360	432	439	446	0.75
7b	$-CH_3$	–Cl	352	352	358	428	443	449	0.72
7c	–OEt	$-CH_3$	340	344	358	443	472	473	0.68
7d	–OEt	–Cl	344	348	354	453	472	480	0.76
7e	–F	$-CH_3$	342	344	350	416	423	424	0.69
7f	–F	–Cl	340	342	348	415	428	738	0.74
7g	–Br	$-CH_3$	346	350	356	406	416	422	0.65
7h	–Br	–Cl	348	348	354	409	420	430	0.68

a) Φ_f: Fluorescence quantum efficiency, relative to 2-phenyl-5-(4-biphenyl)-1,3,4-oxadiazole in benzene ($\Phi_f = 0.80$).

Table 2. Electrochemical Properties of 1,3,4-Oxadiazole–1,2,3-Triazole Derivatives **7a–7h**

Compound	E_{onset}[a] /V	E'_{onset}[b] /V	I_p[c),f] $= E_{HOMO}$ /eV	E_g[d),f] = Bandgap energy/eV	E_a[e),f] $= E_{LUMO}$ /eV
7a	1.21	1.02	−5.63	3.16	−2.47
7b	1.19	1.00	−5.61	3.14	−2.47
7c	1.05	0.86	−5.47	3.13	−2.34
7d	1.15	0.96	−5.57	3.05	−2.52
7e	1.22	1.03	−5.64	3.20	−2.44
7f	1.15	0.96	−5.57	3.20	−2.37
7g	1.35	1.16	−5.77	3.19	−2.58
7h	1.38	1.19	−5.80	3.19	−2.61

a) Measured vs ferrocene/ferrocenium. b) $E'_{onset} = E_{onset} - 0.19$ eV (measured vs Ag/AgCl). c) $I_p = -(E'_{onset} + 4.8)$. d) E_g: the bandgap energy estimated from the onset wavelength of UV–vis absorption. e) $E_a = I_p + E_g$. f) 1 eV = 96.5 kJ mol^{-1}.

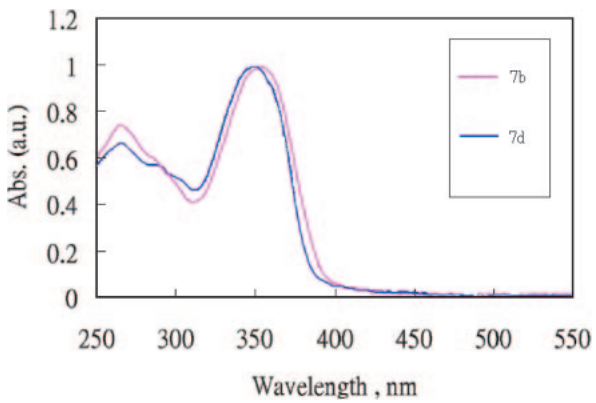

Fig. 1. UV–vis spectra of 1,3,4-oxadiazole–1,2,3-triazole derivatives **7b** and **7d** in THF solution.

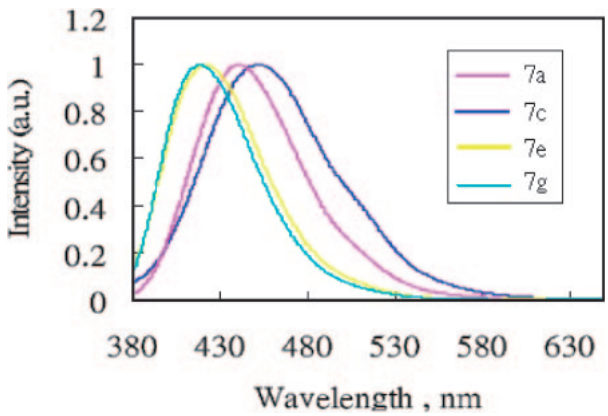

Fig. 2. Normalized photoluminescence spectra of 1,3,4-oxadiazole–1,2,3-triazole derivatives **7a**, **7c**, **7e**, and **7g**.

using a millimolar solution of CH_2Cl_2 containing 0.1 M of the supporting electrolyte, tetrabutylammonium hexafluorophosphate ($TBAPF_6$), in a three electrode cell and potentiostat assembly.[18] The potential was measured against Ag/AgCl as the reference electrode and each measurement was calibrated with an internal standard, a ferrocene/ferrocenium (Fc) redox system.[19] Upon anodic sweep, **7a–7h** showed unclearly reversible reduction processes and the data are tabulated in Table 2. As an example, the cyclic voltammogram of **7c** is shown in Fig. 4. In the case of **7c**, the reversibility of oxidation was estimated with the HOMO value of −5.47 eV with respect to Ag/AgCl (−5.66 eV with respect to Fc). The bandgap energies of the 1,3,4-oxadiazole–1,2,3-triazole derivatives **7a–7h** were estimated from the onset wavelength (λ_{onset}) of the UV–vis absorption.[15] From their high electron affinities, **7a–7h** have earned the potential of being electron-transporting and highly efficient blue electroluminescent materials.

Experimental

Experimental procedure, spectral data, and physical properties of compounds **3a–3d**, **4a–4d**, **5a–5d**, and **6a–6h** are provided in the supporting information section.

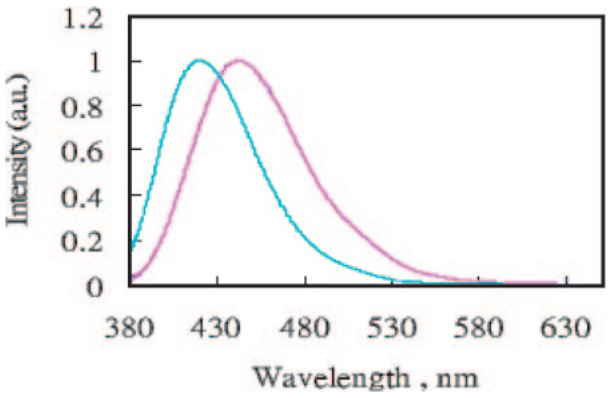

Fig. 3. Normalized photoluminescence spectra of **7h** (blue line: diluted in CH_2Cl_2 solution; red line: vacuum evaporated film).

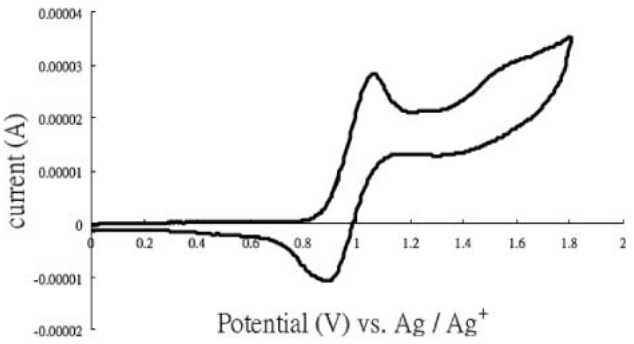

Fig. 4. Cyclic voltammogram of **7c** in CH_2Cl_2 containing 0.1 M $TBAPF_6$ at a scan rate of 50 mV s^{-1}.

Standard Procedure of Dehydration–Cyclization (7a–7h).[10] A solution of 4-[4-(4-substituted phenylamino)-2*H*-1,2,3-triazol-2-yl]-N^2-(4-substituted benzoyl)benzohydrazides (**6a–6h**, ≈230 mg) in $POCl_3$ (10 mL) was stirred at 90 °C for 10 h. After the reaction was completed, cold water (10 mL) was added to the reaction mixture, and the mixture was neutralized with a NaOH aqueous solution (10 mL) to precipitate the reaction product. The product was washed with cold water (5 mL), filtrated and dried in a vacuum oven overnight to give the desired product (**7a–7h**).

2-(4-Methylphenyl)-5-{4-[4-(4-methylphenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-1,3,4-oxadiazole (7a). The standard procedure was followed to prepare **7a** as a white powder in 85% yield: mp 231–233 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 2.24 (s, 3H, CH_3), 2.41 (s, 3H, CH_3), 7.12 (d, J = 8.8 Hz, 2H, Ar-H), 7.40 (d, J = 8.8 Hz, 2H, Ar-H), 7.44 (d, J = 8.0 Hz, 2H, Ar-H), 7.73 (s, 1H, CH), 8.02 (d, J = 8.0 Hz, 2H, Ar-H), 8.12 (d, J = 8.8 Hz, 2H, Ar-H), 8.26 (d, J = 8.8 Hz, 2H, Ar-H), 9.22 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 116.55, 117.16, 118.73, 119.93, 121.64, 125.94, 127.37, 129.23, 132.13, 134.45, 138.16, 142.11, 152.47, 163.78, 164.12; IR (KBr) 3300 (br, NH), 1612 (m, C=O), 1567, 1494, 1432 cm^{-1}; FABMS m/z (relative intensity) 410 (M + 2, 10), 409 (M + 1, 64), 408 (M^+, 48), 155 (19), 154 (94), 138 (33), 137 (51), 136 (100). Anal. Calcd for $C_{24}H_{20}N_6O$: C, 70.57; H, 4.94; N, 20.57%. Found: C, 70.51; H, 4.99; N, 20.55%.

2-(4-Chlorophenyl)-5-{4-[4-(4-methylphenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-1,3,4-oxadiazole (7b). The standard procedure was followed to prepare **7b** as a white powder in 83% yield: mp 229–231 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 2.25 (s, 3H, CH_3), 7.18 (d, J = 8.4 Hz, 2H, Ar-H), 7.42 (d, J = 8.6 Hz, 2H, Ar-H), 7.48 (d, J = 8.2 Hz, 2H, Ar-H), 7.73 (s, 1H, CH), 8.02 (d, J = 8.0 Hz, 2H, Ar-H), 8.15 (d, J = 8.6 Hz, 2H, Ar-H), 8.29 (d, J = 8.4 Hz, 2H, Ar-H), 9.27 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 20.71, 116.30, 117.76, 118.43, 120.63, 122.64, 126.83, 128.86, 129.92, 130.00, 137.17, 139.56, 141.81, 151.23, 162.38, 164.12; IR (KBr) 3301 (br, NH), 1608 (m, C=O), 1565, 1499, 1482, 1432 cm^{-1}; FABMS m/z (relative intensity) 430 (M + 2, 15), 429 (M + 1, 33), 428 (M^+, 23), 155 (19), 154 (100), 138 (33), 137 (66), 136 (98). Anal. Calcd for $C_{23}H_{17}ClN_6O$: C, 64.41; H, 4.00; N, 10.60%. Found: C, 64.40; H, 4.04; N, 10.63%.

2-{4-[4-(4-Ethoxyphenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-5-(4-methylphenyl)-1,3,4-oxadiazole (7c). The standard procedure was followed to prepare **7c** as a white powder in 83% yield: mp 179–180 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 1.31 (t, J = 7.2 Hz, 3H, CH_3), 2.48 (s, 3H, CH_3), 3.99 (q, J = 7.2 Hz, 2H, CH_2), 6.90 (d, J = 8.8 Hz, 2H, Ar-H), 7.54 (d, J = 9.0 Hz, 4H, Ar-H), 7.68 (s, 1H, CH), 8.01 (d, J = 8.7 Hz, 2H, Ar-H), 8.10 (d, J = 8.8 Hz, 2H, Ar-H), 8.24 (d, J = 8.7 Hz, 2H, Ar-H), 9.09 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 15.19, 21.56, 63.59, 115.50, 117.72, 119.78, 120.34, 122.34, 126.32, 127.05, 128.65, 130.39, 137.79, 142.83, 143.18, 151.48, 153.32, 162.38, 164.12; IR (KBr) 3400 (br, NH), 1613 (m, C=O), 1510 cm^{-1}; FABMS m/z (relative intensity) 440 (M + 2, 5), 439 (M + 1, 19), 438 (M^+, 24), 155 (19), 154 (23), 138 (8), 137 (14), 136 (23). Anal. Calcd for $C_{25}H_{22}N_6O_2$: C, 68.48; H, 5.06; N, 19.17%. Found: C, 68.44; H, 5.06; N, 19.15%.

2-(4-Chlorophenyl)-5-{4-[4-(4-ethoxyphenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-1,3,4-oxadiazole (7d). The standard procedure was followed to prepare **7d** as a white powder in 82% yield: mp 288–290 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 1.30 (t, J = 7.2 Hz, 3H, CH_3), 3.97 (q, J = 7.2 Hz, 2H, CH_2), 6.91 (d, J = 8.8 Hz, 2H, Ar-H), 7.33 (d, J = 8.8 Hz, 2H, Ar-H), 7.53 (d, J = 9.0 Hz, 2H, Ar-H), 7.65 (s, 1H, CH), 8.04 (d, J = 8.7 Hz, 2H, Ar-H), 8.08 (d, J = 8.8 Hz, 2H, Ar-H), 8.23 (d, J = 8.7 Hz, 2H, Ar-H), 9.10 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 17.35, 62.55, 115.39, 116.93, 117.22, 121.41, 124.63, 125.83, 126.90, 128.52, 129.75, 132.96, 136.29, 142.11, 152.43, 153.78, 163.84, 164.42; IR (KBr) 3407 (br, NH), 1593 (m, C=O), 1426 cm^{-1}; FABMS m/z (relative intensity) 460 (M + 2, 6), 459 (M + 1, 5), 458 (M^+, 3), 155 (19), 154 (79), 138 (37), 137 (56), 136 (100). Anal. Calcd for $C_{24}H_{19}ClN_6O_2$: C, 62.82; H, 4.17; N, 18.31%. Found: C, 62.91; H, 4.23; N, 18.29%.

2-{4-[4-(4-Fluorophenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-5-(4-methylphenyl)-1,3,4-oxadiazole (7e). The standard procedure was followed to prepare **7e** as a white powder in 82% yield: mp 252–254 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 2.23 (s, 3H, CH_3), 7.25 (d, J = 8.8 Hz, 2H, Ar-H), 7.49 (d, J = 8.7 Hz, 2H, Ar-H), 7.58 (d, J = 8.4 Hz, 2H, Ar-H), 7.66 (s, 1H, CH), 8.07 (d, J = 8.2 Hz, 2H, Ar-H), 8.15 (d, J = 8.2 Hz, 2H, Ar-H), 8.30 (d, J = 8.4 Hz, 2H, Ar-H), 9.42 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 116.25, 117.62, 118.39, 121.10, 122.18, 126.23, 127.36, 128.34, 129.33, 132.49, 133.28, 141.55, 142.93, 151.53, 164.09, 164.78; IR (KBr) 3309 (br, NH), 1606 (m, C=O), 1573, 1507, 1455 cm^{-1}; FABMS m/z (relative intensity) 414 (M + 2, 22), 413 (M + 1, 44), 412 (M^+, 37), 155 (22), 154 (100), 138 (47), 137 (58), 136 (44). Anal. Calcd for $C_{23}H_{17}FN_6O$: C, 66.98; H, 4.15; N, 20.38%. Found: C, 66.97; H, 4.17; N, 20.39%.

2-(4-Chlorophenyl)-5-{4-[4-(4-fluorophenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-1,3,4-oxadiazole (7f). The standard procedure was followed to prepare **7f** as a white powder in 88% yield: mp 265–267 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 7.27 (d, J =

8.4 Hz, 2H, Ar-H), 7.47 (d, $J = 8.4$ Hz, 2H, Ar-H), 7.72 (s, 1H, CH), 7.99 (d, $J = 8.4$ Hz, 2H, Ar-H), 8.08 (d, $J = 8.4$ Hz, 2H, Ar-H), 8.14 (d, $J = 8.2$ Hz, 2H, Ar-H), 8.27 (d, $J = 8.2$ Hz, 2H, Ar-H), 9.36 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 115.13, 117.22, 118.19, 121.05, 123.74, 126.78, 127.11, 128.74, 129.85, 132.19, 132.48, 141.35, 141.69, 150.59, 163.99, 164.42; IR (KBr) 3407 (br, NH), 1593 (m, C=O), 1426 cm^{-1}; FABMS m/z (relative intensity) 434 (M + 2, 19), 433 (M + 1, 40), 432 (M^+, 28), 155 (20), 154 (81), 138 (40), 137 (69), 136 (100). Anal. Calcd for $C_{22}H_{14}ClFN_6O$: C, 61.05; H, 3.26; N, 19.42%. Found: C, 61.11; H, 3.26; N, 19.44%.

2-{4-[4-(4-Bromophenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-5-(4-methylphenyl)-1,3,4-oxadiazole (7g). The standard procedure was followed to prepare **7g** as a white powder in 85% yield: mp 257–259 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 2.41 (s, 3H, CH_3), 7.40–7.52 (m, 6H, Ar-H), 7.76 (s, 1H, CH), 8.03 (d, $J =$ 8.0 Hz, 2H, Ar-H), 8.14 (d, $J = 8.8$ Hz, 2H, Ar-H), 8.27 (d, $J =$ 8.2 Hz, 2H, Ar-H), 9.60 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 20.75, 117.98, 120.16, 120.66, 121.00, 121.73, 125.67, 127.06, 128.67, 129.32, 132.19, 141.37, 142.66, 144.70, 152.53, 165.13, 166.01; IR (KBr) 3310 (br, NH), 1600 (m, C=O), 1559, 1493, 1432 cm^{-1}; FABMS m/z (relative intensity) 475 (M + 2, 21), 474 (M + 1, 19), 473 (M^+, 22), 155 (25), 154 (100), 138 (30), 137 (59), 136 (77). Anal. Calcd for $C_{23}H_{17}BrN_6O$: C, 58.36; H, 3.62; N, 17.75%. Found: C, 58.36; H, 3.25; N, 17.75%.

2-{4-[4-(4-Bromophenylamino)-2*H*-1,2,3-triazol-2-yl]phenyl}-5-(4-chlorophenyl)-1,3,4-oxadiazole (7h). The standard procedure was followed to prepare **7h** as a white powder in 83% yield: mp 261–263 °C; ^{1}H NMR (DMSO-d_6, 300 MHz) δ 7.46 (d, $J = 8.6$ Hz, 4H, Ar-H), 7.71 (d, $J = 8.6$ Hz, 2H, Ar-H), 7.78 (s, 1H, CH), 8.15 (d, $J = 8.6$ Hz, 4H, Ar-H), 8.28 (d, $J = 8.6$ Hz, 2H, Ar-H), 9.55 (s, 1H, NH); ^{13}C NMR (DMSO-d_6, 75 MHz): δ 115.63, 118.33, 119.09, 120.60, 124.24, 127.07, 127.83, 129.53, 130.17, 131.84, 141.62, 142.73, 143.79, 152.37, 163.44, 164.37; IR (KBr) 3313 (br, NH), 1605 (m, C=O), 1560, 1484 cm^{-1}; FABMS m/z (relative intensity) 495 (M + 2, 26), 494 (M + 1, 24), 493 (M^+, 21), 155 (26), 154 (100), 138 (33), 137 (63), 136 (75). Anal. Calcd for $C_{22}H_{14}BrClN_6O$: C, 53.52; H, 2.86; N, 17.02%. Found: C, 53.55; H, 2.86; N, 17.03%.

Conclusion

We were successful in introducing a triazole moiety into the skeletal structure of 1,3,4-oxadiazole to provide a series of new potential blue electroluminescent materials. The triazole moiety plays an excellent role as an asistant in controlling fundamental photolytic processes.

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Supporting Information

Experimental procedures and characterization data for new compounds. This material is available free of charge on line at http://www.csj.jp/journals/bcsj/.

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