Achieving Diversified Emissive Behaviors of AIE, TADF, RTP, Dual-RTP and Mechanoluminescence from Simple Organic Molecules by Positional Isomerism

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Abstract: Organic emitters with multiple emissions such as aggregation-induced emission (AIE), thermally activated delayed fluorescence (TADF), room-temperature phosphorescence (RTP), and mechanoluminescence (ML) are promising candidates for various high-tech applications but still very rare. Here, for the first time, an effective strategy of positional isomerism is applied to obtain simple organic isomers featuring diversified emissive behaviors of AIE, TADF, RTP, dual-RTP, and ML. In Particular, simultaneous AIE, TADF, and ML are

successfully realized in the *ortho*-isomer *o*-CITPA while typical AIE and unique dual-RTP coexist in the *para*-isomer *p*-CITPA. Crystal structure analysis shows that the subtle variation in the substitution position can significantly alter intermolecular interactions and molecular packings, which in turn exerts remarkable effects on crystal-state emissive properties. Therefore, diversified emissive behaviors of TADF, RTP, dual-RTP, and ML are consequently observed from these positional isomers. Furthermore, theoretical calculations not only afford deep insight into the mechanism of different luminescent properties but also elaborate the relationship between positional isomers featuring diversified emissive behaviors of AIE, TADF, RTP, dual-RTP, and ML are reported for the first time, which will deepen the understanding of the relationship between molecule structures and multiple emissions.

1. Introduction

Metal-free organic materials with multifarious luminescent properties have attracted considerable attention because of their promising applications in the fields of organic lightemitting diodes (OLEDs), sensors, biological imaging, and anti-counterfeiting.^[1-4] As we know, the bulk properties of organic materials used in the real world are not just governed by the properties of a single molecule but also by its packing modes.^[5-6] However, most conventional chromophores with planar configuration suffer from the notorious aggregation-caused quenching (ACQ) effect upon aggregation.^[7] Until 2001, Tang and co-workers firstly coined the concept of aggregation-induced emission (AIE), which is diametrically opposed to the ACQ effect.^[8] The AIE luminogens (AIEgens) are weakly or non-emissive as free molecules but show remarkably enhanced emission when aggregated. Owing to this unique advantage, AIEgens have been widely used in various high-tech applications in the past two decades.^[9]

Recently, some exciting luminescent properties such as thermally activated delayed fluorescence (TADF), room-temperature phosphorescence (RTP), and mechanoluminescence (ML) have been successfully achieved in certain AIEgens.^[10-13] It should be noted that TADF and RTP are two pathways to harvest "dark" triplet states for potential applications in the optoelectronic and biological areas while stimuli-responsive ML is promising for smart sensing and switching devices. To obtain desirable emission properties and hence fulfill the requirements for versatile practical applications, enriching the diversity of excellent chromophores by molecule engineering is of significant importance. Over the past decades, various strategies such as changing the position of substituents^[9f,14], tailoring the length of alkyl chains^[15], altering the central core, and introducing functional groups^[16] have been devised to modify the molecular structures, thus tuning the electronic structure or molecular packing motif

to obtain diverse luminescent properties. Except for the intrinsic electronic structure, intermolecular interactions and molecular packings also play crucial roles in tailoring the luminescent behaviors of organic aggregates.^[17-18] Accordingly, in addition to chemical modifications, physical treatments such as light irradiation, heating, applying mechanical force, and changing solvent polarity have been widely used to realize dynamic emission behaviors ^[19] So far, although organic materials with different emissive properties such as AIE, TADF, RTP, and ML have been developed well independently^[9f,13], how to rationally design and tailor the molecular structure within macroscopic aggregates to obtain desired emission properties remains a big challenge.

Integrating diverse emissive properties such as TADF, RTP, and ML into a single molecule has emerged as attractive candidates to unveil new mechanisms and extend versatile applications.^[20-24] However, it is extremely challenging to balance different radiative transitions in a single molecule. Until recently, Yang and co-workers firstly reported a simple organic molecule showing simultaneous AIE, TADF, RTP, and ML properties.^[25] Excitedly, Chi et al. designed a soft organic molecule with multiple emissions of TADF, RTP, and ML by selectively expressing chromophores.^[26] Despite these excellent works, multifunctional organic emitters are still very scarce partly due to the lack of reliable guidance. Meanwhile, the abovementioned multifunctional organic emitters are found serendipitously because it is tricky to obtain various kinds of crystals from one single molecule. Herein, we focus on studying the solid-state luminescence of basic dyes to develop multifunctional organic materials with simple structure and easy accessibility. Triphenylamine (TPA) is a promising candidate in this context because it exhibits a simple propeller-shaped structure and is susceptible to further modifications. Furthermore, positional isomerism, a fundamental concept in organic chemistry, can remarkably influence the physicochemical properties of organic molecules.^[27] Indeed, a minor change in the substitution position has been demonstrated to drastically influence the optoelectronic properties of organic semiconductors.^[28] Nevertheless, the role of positional isomerism in controlling the excited-state properties is less developed. With these in mind, we have designed three simple positional isomers with the Cl group located in the ortho-, meta-, and para-positions on the TPA core, respectively (Figure 1). These isomers can be easily prepared via the same one-step reaction from commercially available raw materials. Meanwhile, the ester and Cl groups can not only promote the spin-orbit coupling (SOC) between the singlet and triplet states but also facilitate the intramolecular charge transfer (CT) to regulate tripletexciton behaviors. Experimental results show that although the three isomers have similar photophysical properties in dilute solutions, diversified emissive behaviors of typical AIE,

TADF, ML, RTP and unique dual-RTP are successfully realized in crystals (Table 1). In particular, the *ortho*-isomer achieves simultaneous AIE, TADF, and ML properties while typical AIE and unique dual-RTP coexist in the *para*-isomer. The crystal structure analysis reveals that a slight difference in the substitution position can significantly alter intermolecular interactions and molecular packings, which in turn drastically impacts excited-state electronic structures and thus emissive properties in crystals. Theoretical studies not only reveal the emission mechanisms of TADF, RTP, and dual-RTP of these isomers but also unveil the crucial contributions of intermolecular interactions and molecular packings rather than intrinsic excited-state electronic structures to the diversified emissive behaviors in the crystal state. This work elaborates the underlying reasons for the significantly different effect of positional isomerism on the luminescent properties in solution and crystal states of simple isomers, which could aid in designing multifunctional organic materials.



Figure 1. The chemical structures of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA, and their corresponding luminescent properties in dilute solution and crystal states, respectively.

2. Results and Discussion

Positional isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA are readily synthesized by the same one-step reaction in medium yields (Scheme S1) and thoroughly characterized by ¹HNMR, ¹³CNMR, high-resolution mass spectroscopy, single-crystal X-ray diffraction, elemental analyses, and high-performance liquid chromatography. Despite simple structures, melting points on the differential scanning calorimetry (DSC) curves of the three isomers are estimated to be 151.9, 118.1, and 160.7 °C for *o*-CITPA, *m*-CITPA, and *p*-CITPA, respectively. (Figures S1). These high melting points are indicative of strong intermolecular interactions which are conducive to suppressing non-radiative relaxations.

	Solutions					Crystals						
Isomers	λ_{onset}	λ_{ab}	λ_{F}	λр-77 к	τр-77 к		λ_{F}	τ_{F}	λ_{d}	τ_{d}	λ_{ML}	Φ_{PL}
	(nm)	(nm)	(nm)	(nm)	(ms)		(nm)	(ns)	(nm)	(ms)	(nm)	(%)
o-CITPA	405	296	443	470	247.7	460	16.89	462	0.56	460	41.3	
		350										
<i>m</i> -CITPA	418	299	437	475	312.6	447	3.23	496	0.74	1	9.45	
		360								,		
<i>p</i> -CITPA	425	301	452	482	277.3		462	2 76	472	0.81	/	9 54
		370	-102	-102			2.70	535	1.23	,	0.04	

Table 1. Summary of photophysical parameters of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA in dilute solutions and crystals, respectively.

^{a)} λ_{onset} : onset absorption; λ_{ab} : absorption peaks; λ_F : fluorescent emission peak; $\lambda_{P-77 \ K}$: phosphorescent emission peak at 77 K; $\tau_{P-77 \ K}$: phosphorescent lifetime at 77 K; λ_d : delayed emission peak; τ_F : fluorescent lifetime; τ_d : the lifetime of delayed emission; λ_{ML} : mechanoluminescence peak; Φ_{PL} : total photoluminescence quantum yield.



Figure 2. (A) UV-vis absorption and (B) steady-state PL spectra of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA in dilute THF solutions (10^{-5} M) at room temperature; (C) prompt and delayed PL spectra and (D) transient delayed PL decay curves of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA in dilute THF solutions at 77 K; (E) prompt and delayed PL spectra of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA in crystals at room temperature; (F) PL and ML spectra of *o*-CITPA in crystals (inset: ML image in the dark); (G) transient delayed PL decay curves of isomers *o*-CITPA, *m*-CITPA, *m*-CITPA, and *p*-CITPA in crystals at room temperature.

Firstly, the photophysical properties of these isomers are studied in dilute THF solutions. As illustrated in Figure 2A, the three isomers display similar absorption spectra with two sets of absorption bands in the range of $250 \sim 450$ nm, which can be attributed to the locally-excited (LE) and intramolecular charge transfer (ICT) transitions, respectively.^[25, 29] Owing to the

reduced steric hindrance resulting from the subtle variation in the substitution position of the Cl atom, the ICT absorption band is gradually redshifted from o-MCBA to m-MCBA and then to *p*-MCBA. Likewise, the three isomers also show similar fluorescence spectra with a broad and featureless emission band originating from the radiative transition of the CT excited state (Figure 2B). Additionally, when the polarity of the THF/water mixture is gradually increased by progressively increasing the water fraction, the fluorescent emission of these isomers is gradually redshifted with reduced intensity (Figure S2). Until a high water fraction (99%), the fluorescence emission is blueshifted with enhanced intensity due to the formation of aggregates. These phenomena are indicative of typical twisted ICT (TICT) and AIE characteristics of these isomers, which is consistent with their twisted donor-acceptor structures.^[30] Meanwhile, the dependence of the fluorescent emission on the solvent polarity, along with scanning electron microscope (SEM) images and dynamic light scattering (DLS) results under different water fractions further confirms the TICT and AIE characteristics of these isomers (Figure S3-S5). Besides, these isomers show persistent afterglow in dilute solutions at the low temperature of 77 K. As shown in Figure 2C, the three isomers exhibit very similar low-temperature phosphorescence spectra with maximum emission peaks located at 470, 475, and 482, respectively. By fitting the delayed emission decay curves, ultralong lifetimes of 247.4, 312.6, and 277.3 ms are estimated for o-CITPA, m-CITPA, and p-CITPA respectively (Figure 2D), indicating that molecular motions are efficiently restricted under cryogenic temperatures. These experimental results in dilute solutions demonstrate that positional isomerism has a slight impact on the photophysical properties of these isomers at the molecular level.

Despite similar photophysical properties in dilute solutions, the three isomers show quite different emissive properties in crystals. As illustrated in Figure 2E, the prompt and delayed PL spectra of *o*-CITPA are almost identical, which is suggestive of the delayed fluorescence feature. As for *m*-CITPA, a remarkable redshift is occurred between the prompt and delayed PL spectra, which is indicative of typical RTP property. By fitting the prompt and delayed PL decay curves of isomers *o*-CITPA and *m*-CITPA, nanoseconds and milliseconds lifetimes are estimated for the prompt fluorescence and delayed fluorescence or phosphorescence, respectively (Figure 2G and Figure S6), further confirming their delayed fluorescence and RTP properties in crystals. Interestingly, a dual-emission band appears on the delayed PL spectrum of *p*-CITPA, which is redshifted ~ 10 nm from the emission band on the prompt PL spectrum. Moreover, different milliseconds lifetimes are estimated for the two peaks composing of the dual-emission band (0.81 ms@470 nm and 1.23 ms@535 nm), indicating that this dual-emission band could be ascribed to the dual-RTP originated from the radiative decays of different triplet states (*e.g.*, T₁)

and T₂). With temperature cooling to 77 K, the lifetime of the long-wavelength emission peak is increased two orders of magnitude while that of the short-wavelength emission peak is raised only eight folds (Figure S7, 6.3 ms@470 nm, 167.6 ms@535 nm). Also, with the temperature gradually decreasing from room temperature to 77 K, the long-wavelength emission peak is gradually intensified while the short-wavelength emission peak is slightly changed (Figure S8). These results further verify the dual-RTP property of *p*-CITPA in crystals, because the shortwavelength peak can be assigned to the radiative transition from the upper-lying T₂ state populated from the T₁ state under thermal activation.^[31-33] In contrast, with the temperature gradually increasing from 77 K to room temperature, the phosphorescence emission peak at ~ 515 nm is gradually weakened and eventually replaced by the delayed fluorescence peak at ~ 460 nm and gradually intensified. This result reveals that the delayed fluorescence of o-ClTPA can be attributable to the TADF which is occurred via efficient RISC under thermal activation. Interestingly, upon scratching the crystals of the three isomers by a metal rod, only o-CITPA can emit bright blue light without UV irradiation, which is indicative of the unique ML property of o-CITPA in crystals (Video 1). As shown in Figure 2F, the ML and PL spectra of o-CITPA are overlapped well with each other, implying that the ML is stemmed from the intrinsic fluorescence of o-CITPA rather than other species. It should be noted that the much higher photoluminescence quantum yield of o-CITPA among the three isomers also contributes to the simultaneous TADF and ML properties in the crystal state because of reduced nonradiative relaxations (Table 1). These experimental results demonstrate that the subtle variation in the substituent position has a profound impact on the luminescent properties of these isomers at the aggregate level.

Table 2	Summary o	of inte	ermolecular	r inter	ractions	in tl	ne single-crys	stal structur	res o	f isomers	0-
CITPA,	<i>m</i> -ClTPA,	and	<i>p</i> -ClTPA	(the	figures	in	parentheses	represent	the	number	of
intermol	ecular intera	action	ıs).								

Intermolecular interactions	o-CITPA	<i>m</i> -CITPA	<i>p</i> -CITPA
(Ar) C-Hπ	2.844 Å (2)	2.880 Å (2)	
	2.292 Å (2)	2.598 Å (2)	
(AI) C-HO-C	2.603 Å (2)	2.716 Å (2)	
(Ar) H-CO=C	3.211 Å (2)		
(Ar) C-HC=O			2.779 Å (4)
(Ar) C-HH-C (Ar)			2.273 Å (2)
(CH ₃) C-HCl	2.883 Å (2)		
(CH ₃) C-HO=C		2.591 Å (2)	



Figure 3. (A-B) Molecular geometries of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA in the gas and crystal phases, respectively; (C-D) intermolecular interactions and molecular packing styles in the single-crystal structures of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA, respectively.

Given that these isomers display similar photophysical properties at the molecular level, single-crystal structure analysis is performed to understand the impact of intermolecular interactions and molecular packings on their crystal-state luminescent properties. As depicted in Figure 3A, these isomers show similar distorted molecular geometries in the gas phase, which become different but less distorted in the crystal phase due to the positive effect of intermolecular interactions and molecular packings. Indeed, different types of intermolecular interactions are formed in the crystal structures of these isomers (Table 2). As illustrated in Figure 3C, a single *o*-CITPA molecule is involved in ten intermolecular interactions including C–H···π (2.844 Å), C–H···Cl (2.883 Å), C-H···O=C (2.292, 2.603 Å), and H-C···O=C (3.211 Å). Under these abundant intermolecular interactions, o-CITPA adopts a compact packing mode which is conducive to suppressing nonradiative decays. In contrast, fewer intermolecular interactions exist in isomers *m*-ClTPA and *p*-ClTPA. Consequently, *m*-ClTPA exhibits a loose packing style due to the existence of a freely rotatable phenyl unit, but a much tighter and ordered molecular arrangement is formed in p-CITPA due to the symmetric molecular configuration. In addition, the melting pointing of *p*-ClTPA is much higher than *m*-ClTPA (Figure S1), which also indicates the stronger intermolecular interactions of *p*-ClTPA in crystals. We assume that the stronger intermolecular interactions of *p*-CITPA in crystals are beneficial

to restrict molecular motions and thus stabilize the higher T_2 state for the realization of dual-RTP emission. Besides, although the crystal structures are all centrosymmetric (Table S1), the molecular dipole moment of *o*-CITPA is calculated to be the largest among the three isomers (Figure S9). Therefore, the synergy of large dipole moment, abundant intermolecular interactions, and tight packing motif should be responsible for the distinctive ML behavior of *o*-CITPA in crystals.



Figure 4. (A-B) Calculated energy level diagrams, spin-orbit coupling (SOC) constants between the involved S_n and T_n states (ξ_{S1-Tn} , ξ_{S2-Tn} , ξ_{S0-T2} , ξ_{S0-T1}) of isomers *o*-ClTPA, *m*-ClTPA, and *p*-ClTPA in the gas and crystal phases, respectively; (C) emission mechanisms of TADF, RTP, and dual-RTP of isomers *o*-ClTPA, *m*-ClTPA, and *p*-ClTPA, respectively.

To reveal the mechanism of diversified emissive behaviors and establish the structureproperty relationship, the density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations are performed on the three isomers in the gas and crystal phases, respectively. As shown in figure 4A, in the gas phase, the three isomers have similar energy level diagrams, as well as the energy splitting (ΔE_{ST}) and SOC constants (ξ_{S1-Tn}) between the lowest singlet state (S₁) and involved triplet states (T_n). Especially, this relatively large ξ_{S1-Tn} and small ΔE_{ST} are conducive to generating triplet excitons via promoting ISC, thus activating the low-temperature phosphorescence of isolated molecules in dilute solutions. Meanwhile, these isomers display similar HOMO and LUMO distributions because of their similar optimized molecular configurations (Figure S10). The natural orbital transitions (NOTs) analysis indicates that the three isomers display extremely similar transition configurations of $S_0 \rightarrow S_1$ and $S_0 \rightarrow T_1$, mainly composed of the HOMO→LUMO component (Figure S11). These qualitative and quantitative calculations manifest those similar luminescent properties of these isomers in dilute solutions can be ascribed to their similar excited-state electronic structures and transition configurations. However, the energy level diagrams of these isomers become quite different in the crystal phase (Figure 4B). Particularly, the energy splitting between the S₁ and S₂ (ΔE_{S1-S2}) is large of up to 1.07 eV in o-CITPA. According to the energy-gap law, ^[34-36] the large ΔE_{S1-S2} would lead to comparatively slow IC from the S₂ to S₁ due to small horizontal Franck-Condon factors, and multiple ISC channels ($S_2 \leftrightarrow T_n$ and $S_1 \leftrightarrow T_n$) are available to facilitate the population of triplet states in o-CITPA. Likewise, the energy splitting between the T₁ and T₂ (ΔE_{T1-T2}) is large of 0.70 eV which would largely restrict the IC from the T₂ to T₁. Under the cooperation of large ΔE_{S1-S2} and ΔE_{T1-T2} values, as well as relatively large SOC constant between the S₁ and T₂ states (0.85 cm^{-1}) , the reverse ISC (RISC) from the higher T₂ to S₁ could successfully proceed by competing with the restrained IC from the T_2 to T_1 . On the other hand, the small energy gap between the T_2 and T_1 (0.24 eV) is also favorable for the efficient RISC from the T_1 to S_1 . Consequently, the delayed fluorescence of o-CITPA is emitted from the radiative decay of S₁ excitons regenerated via RISC from both T2 and T1 under thermal activation. In comparison to the isomer o-CITPA, the smaller ΔE_{S1-S2} values (0.72 and 0.78 eV) and fewer triplet states lying below the S₂ would lead to fewer and less efficient ISC processes to populate T₂ excitons in isomers *m*-CITPA and *p*-CITPA. Meanwhile, due to the smaller ΔE_{T1-T2} values (0.49 and 0.54) eV) and SOC constants between the S_1 and T_2 states (0.50 and 0.51 cm⁻¹), the RISC from the higher T_2 to S_1 could not compete with the fast IC from the T_2 to T_1 . Furthermore, the SOC constants from T_1 to S_0 (1.73 and 1.72 cm⁻¹) are large enough, which could guarantee the radiative decay rate of T₁ for phosphorescence emission in isomers *m*-CITPA and *p*-CITPA. It should be noted that the SOC constants from T_2 to S_0 (ξ_{S0-T2}) are larger than those from T_1 to S_0 , which makes it possible to observe the dual-RTP emission from both T_1 and T_2 in the crystals of isomers *m*-CITPA and *p*-CITPA. However, due to the weaker intermolecular interactions and loose packing style, the dual-RTP emission is not realized in the crystals of m-CITPA. Besides, the HOMO and LUMO distributions of o-CITPA are quite different from those of isomers *m*-CITPA and *p*-CITPA (Figure S12). As a result, the NOTs of S_1 and T_1 states mainly composed of HOMO→LUMO transitions are also different (Figure S13), which is consistent with the different emission mechanisms of the three isomers. These theoretical calculations not only reveal the mechanism of different emissive properties of these isomers in the crystal state but also the underlying reason for the remarkably different effects of positional isomerism on the solution- and crystal-states luminescent properties.



Figure 5. (A-C) Simulated UV–vis absorption, and emission spectra of the S₁ and T₁ states of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA in the THF phase; (D) simulated emission spectra of S₁ and T₁/T₂ states of isomers *o*-CITPA, *m*-CITPA, and *p*-CITPA in the crystal phase.

Finally, we also simulate the absorption and emission spectra of the three isomers in the THF solution and crystal phases, respectively. As shown in Figure 5A, the three isomers display similar absorption spectra on which the ICT band is also gradually redshifted from o-CITPA to m-CITPA and then to p-CITPA, agreeing well with experimental results obtained in dilute THF solutions. Likewise, similar structureless emission bands appear on their simulated fluorescence spectra (Figure 5B), and the relative position of these structureless emission bands is consistent with experimental results. However, the simulated phosphorescence spectra of these isomers in the THF phase vary greatly from experimental results (Figure 5C). This is because the low-temperature effect is not involved in the simulation process due to the calculation complexity and poor accuracy. Satisfyingly, the fluorescence and phosphorescence spectra simulated for the three isomers in the crystal phase are in good accordance with experimental results. Specifically, there is a good overlap between the emission spectra of S₁ and T₁ states in m-CITPA, further confirming their TADF and RTP properties in crystals, respectively. As for p-CITPA, the dual-emission band composed of T₂ and T₁ states is slightly redshifted from

the emission spectrum of the S_1 state, which not only verifies its dual-RTP emission in the crystal state but also attributes the dual-RTP to the radiative transitions from the T_2 and T_1 states, respectively.

3. Conclusion

In summary, we have designed three simple isomers which are readily synthesized by the same one-step reaction by locating the Cl group on the ortho-, meta- and para-positions of phenyl unit, respectively. In dilute solutions, these isomers show similar fluorescence and lowtemperature phosphorescence properties, which is indicative of the insignificant effect of positional isomerism on the emissive behaviors of isolated isomeric molecules. In contrast, these isomers exhibit diversified emissive behaviors of AIE, TADF, RTP, dual-RTP, and ML in crystals, among which simultaneous AIE, TADF, and ML properties are realized in o-ClTPA while unique dual-RTP and typical AIE characteristics coexist in *p*-ClTPA. Moreover, crystal structure analysis and theoretical calculations reveal that distinctive intermolecular interactions and molecular packings should be responsible for diversified luminescent properties of the three isomers in the crystal state given that these isomers have similar intrinsic excited-state electronic structures. Of note, the TADF property of ortho-isomer is attributable to the favorable RISC from the higher T₂ to the S₁ while its distinctive ML among the three isomers is endowed by the large molecular dipole moment and strong intermolecular interactions with a tight molecular packing motif. More importantly, emission spectra of singlet and triplet states simulated for these isomers in the crystal phase agree well with experimental results, which further verifies the TADF, RTP, and dual-RTP properties of isomers o-CITPA, m-CITPA, and *p*-CITPA, respectively. To the best of our knowledge, simple organic isomers featuring diversified emissive behaviors of AIE, TADF, RTP, dual-RTP, and ML in the crystal state through the subtle variation in the substitution position are reported for the first time, demonstrating the importance of positional isomerism for tunable photophysical properties within molecular aggregates.

[CCDC 1816586, 1816585, and 1816587 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.]

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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