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Head-to-Tail interlocking aromatic rings of a hydrazine functionalized Schiff base for the development of Nano-aggregates with blue emission: Structural and spectroscopic characteristics



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ABSTRACT

We report the synthesis, physicochemical and morphological characterisation, supramolecular interactions and aggregation-induced blue emission of a newly developed Schiff base, 1,2-bis(phenyl(pyridin-2-yl)methylene)hydrazine (P18). The compound was synthesised through a condensation reaction between hydrazine and 2-benzoylpyridine under reflux in ethanol. The photophysical behaviour of the Schiff base was studied in both monomeric and aggregated forms. Interestingly, the molecular aggregate showed a significant blue shift with ~ 20 fold higher fluorescence intensity with lifetime, 0.99 ns in the aqueous phase than that of monomeric form, attributed to the development of J-type aggregation. The crystal structure, C-H $\cdots\pi$ and π ... π interactions, were enumerated to decipher the nature of aggregation. The Schiff base consisting of four aromatic rings (two pyridine and two phenyl rings) displayed a short C- $H \cdots \pi$ and a long distant $\pi \cdots \pi$ interactions causing a head-to-tail type interlocking of aromatic rings. Energy framework analysis confirmed the predominance of dispersive forces (-192.4 kJ/mol) to the cluster of molecules, thus playing a significant role in the restriction of intramolecular motion of the aromatic rings of P18. A restrain on the rotational probability of = N-N = and Ar-C- bonds leads to an enhancement of an intense fluorescence property of nano-aggregate with blue light emission in solid state. The propagation of the rectangular-shaped monomeric probe in the nano-aggregate with an average hydrodynamic size of 270(±3) nm was established with field emission scanning electron microscopy, dynamic scattering light, and electron dispersive X-ray spectral analysis.

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1. Introduction

The advancement of functional luminophores in light-emitting and light-harvesting processes shows a great promise in bringing novel characteristics and properties to the materials [1,2]. The evolution of light-dependent molecular devices and technologies has triggered a paramount interest to material scientists for the indispensable contribution of molecular devices in scientific and societal advancement [3]. In this context, molecular aggregation beyond the microscopic level is a highly fascinating phenomenon that attributes novel properties to functional materials and the design of high-tech photo-electronic devices [4–6]. Nowadays, the aggregation-induced emission (AIE) phenomenon provides an exciting avenue in scientific research to unveil the properties of

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molecular aggregate [1–3]. The advent of newly developed properties endowed by molecular aggregates introduces new characteristics and functionalities in the molecular aggregate compared to single molecules [3,4,7].

AlE deals with a class of molecules having dim or low emission properties in dilute solution. However, the compounds display a pronounced effect on enhancing emission properties in molecular aggregates [8]. A systematic study by Tang *et al.* on different AlE systems summarises that the restriction of active intramolecular motion in the molecular aggregate limits the excited-state nonradiative decay. In contrast, dynamic intramolecular motion increases the non-radiative decay and quenches the molecular emission [9]. Further, the motion-responsive molecular aggregates exhibit strong emission properties in solid state, enabling unique applications in different dimensions, including chemical sensors, fluorescent imaging, photonic drugs, bio-probes, optoelectronics and others [4–7,10].



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Typically, azines contain aromatic units bridged through rotatable N–N bonds and are the highly stable condensation products of carbonyl compounds and hydrazine [14,15]. Azine compounds show an excellent promise for their straightforward synthetic approach, high yield and easy isolation of the products, costeffective, high stability to apply for suitable technological applications and devices [11–13]. In general, H-type aggregation induces a non-radiative deactivation process, while the J-type aggregation imparts a relatively high fluorescence efficiency [16–18].

Intermolecular non-covalent interactions involving aromatic systems are considered emerging inductors to develop a vast array of long-range crystalline architectures through crystal engineering [19–22]. Different weak forces such as hydrogen bonding, $\pi \cdots \pi$ and C-H··· π short contacts in crystalline materials are imperative to design new materials with novel properties [23,24]. Therefore, the proper understanding of weak forces allows envisioning the role of supramolecular assemblies in developing novel functional properties [25,26]. It is evident that weak intermolecular forces have a pronounced effect on AIE property and, eventually, may bring a substantial change in the size and phase of crystalline materials [27,28]. Herein, we report the design and synthesis of an azine type Schiff base and explore its aggregation behaviour with a suite of spectroscopic and crystallographic studies. The dominant dispersive forces significantly stabilise the cluster of molecules and mingle the aromatic rings through the head to tail type interlocking. This phenomenon imposes a strict restriction on the intramolecular rotation and vibration of aromatic rings in the Schiff base with the development of blue emission.

2. Experimental

2.1. Chemicals, solvents and starting materials

>99% pure 2-benzoylpyridine (Aldrich, USA) and > 98% pure hydrazine monohydrate (TCI, Japan) were procured from the respective commercial sources. All the chemicals and solvents were of spectroscopic grade and used as received.

2.2. Preparation of Schiff base

The Schiff base was prepared following a reported synthetic procedure with a little modifications [29–32]. The Schiff base was synthesised by refluxing 2-benzoylpyridine (0.3660 g, 2 mmol) with hydrazine monohydrate (0.050 g, 1 mmol) in 30 mL ethanol for 10 h. The reaction solution was filtered and dried. The compound was stored *in vaccuo* over CaCl₂. Yield: 0.360 g (~86.50%). Anal. Calc. for C₂₄H₁₈N₄ (**P18**): C, 79.54; H, 5.01; N, 15.46; Found: C, 79.58; H, 5.05; N, 15.50. IR (KBr, cm⁻¹; Fig. S1): 1624, 1582 ($v_{C=N}$); ¹H NMR (δ ppm, 400 Mz, DMSO *d*₆; Fig. S2) δ = 8.702–6.6 17 (Ar–H, 18H), ¹³C NMR (400 MHz, Fig. S3): 158.34–121.11; MALDI TOF MS (*m*/*z*, Fig. S4): 362.48 (Expt.); UV–Vis (λ_{max} , nm; Fig. S5): 263 (0.433), 285 (0.383);

2.3. Physical Measurements

The infrared spectrum of the compound was recorded with an FTIR-8400S SHIMADZU spectrophotometer in the range 400–3600 cm⁻¹. The ¹H and ¹³C NMR spectra of P18 were obtained on a Bruker Advance 400 MHz spectrometer at 25 °C. The MALDI TOF mass spectrum of the Schiff base was recorded using a Q-tof-micro quadruple mass spectrometer. All the ground-state absorption spectra were recorded on a JASCO V-730 UV–Vis spectrophotometer, and the fluorescence spectra were measured on a Hitachi F-7000 spectrofluorometer. Elemental analyses were carried out on a Perkin Elmer 2400 CHN microanalyser.

2.4. Crystal structure determination, refinement and Hirshfeld surface analysis

The Schiff base's single crystal X-ray diffraction data were collected on a Rigaku XtaLABmini diffractometer equipped with Mercury 375R (2 × 2 bin mode) CCD detector. The data were collected with graphite monochromated Mo-K α radiation (λ = 0.71073 Å) at 100 K using ω scans. The data were reduced using CrysAlisPro 1.171.39.35c [33], and the space group determination was done using Olex2. The structure is resolved by the dual space method using SHELXT-2015 and refined by full-matrix least-squares procedures using the SHELXL-2015 [34,35] software package through the OLEX2 suite [36]. The Crystal Explorer17.5 [37] programme was used to generate Hirshfeld surfaces and 2D fingerprint plots of the Schiff base. The details of the analysis are reported elsewhere [38,39].

2.5. Preparation and characterisation of the molecular aggregate

A stock solution of 1.020 mM P18 was prepared in a DMSO medium. 20 μ L of the DMSO solution of P18 was injected into 2 mL of Milli-Q-water and kept undisturbed for 10 mins at room temperature. The molecular aggregate of P18 was developed following the drop-casting method and recorded the Field Emission Scanning Electron Microscope (FESEM) images on a clean aluminium foil. FESEM images and the electron dispersive X-ray (EDX) plot were recorded with a JSM-6700F FESEM, JEOL, Japan instrument, which confirmed the nature of molecular aggregate in the solid state. The dynamic light scattering (DLS) study of the aggregation study in an aqueous medium was carried out at 25 $^{\circ}$ C on a Malvern Instrument with Zetasizer Nano ZS90 instrument. The hydrodynamic size of the P18 was measured by adding 100 μ L of P18 solution to 1.5 mL of water and recorded in triplicate to find an average number size distribution.

3. Results and Discussion

3.1. Synthesis of the Schiff base

The Schiff base was synthesised through the condensation reaction between hydrazine and 2-benzoyl pyridine in ethanol and under refluxing conditions for 8 h (Scheme 1). The method of recrystallisation was employed to develop the single crystals in methanol. The schematic synthetic route is shown below.

3.2. Spectroscopic characterisation of P18

Different spectroscopic and analytical methods were used to determine the molecular structure and its structural characteristics. The FT-IR spectrum of the Schiff base showed characteristic stretching vibrations (Fig. S1) at 1624 and 1582 cm⁻¹ which were assignable to the azomethine group of the Schiff base. Other peaks at 1460 and 1349 cm⁻¹ for P18 attributed to -C = C- groups in the Schiff base. These appearances of the characteristic peaks resemble very well with the previously reported values [40,41].

The NMR spectral analysis of P18 was carried out in DMSO d_6 . Figs. S2 and S3 displayed the ¹H and ¹³C NMR spectra of P18, respectively. The appearance of the protons signals in the range 8.70 to 6.61 ppm corresponded to the aromatic-H of phenyl and pyridine rings for P18 (Fig. S2). The characteristic C-signals of P18 were observed from 159.64 to 121.11 ppm in the ¹³C NMR spectra (Fig. S3) which confirmed the presence of azomethine-C and aromatic-C atoms. The dense-splitting patterns of the signals were attributed to the presence of Ar-H and Ar-C in P18 and portrayed a pure signature for the existence of non-covalent



Scheme 1. Preparation method of the Schiff base.

interactions as previously evident from the report of Zhao et al. [42]. The MALDI TOF mass spectrum was also recorded for P18 at room temperature, which confirmed the presence of molecular ion peak at m/z 362.4837 (Fig. S4). The absence of any other peaks in the mass spectrum ensures the absence of the impurities in the solution.

The electronic spectra of P18 were recorded in aqueous and DMSO media in the 200–900 nm range. The electronic spectrum of P18 in DMSO showed blue-shifted electronic bands than those in the aqueous medium. P18 exhibited characteristic absorption bands at 263 and 285 nm (Fig. S5), attributing the intra-ligand $\pi - \pi^*/n - \pi^*$ electronic transitions of the P18 probe. The reported electronic bands for P18 were in well-agreement with the reported values [43].

The steady-state fluorescence spectrum of P18 in an aqueous medium was also recorded and shown in Fig. S6. The emission maximum for P18 was observed at 300 nm with low intensity. The nature of the fluorescence spectrum suggests its mild fluorescence properties in the aqueous medium at room temperature.

3.3. Microscopic analysis of the aggregate of Schiff base

The FESEM images of the aggregated form of P18 (Fig. 1a) were recorded to study the aggregation properties of the monomeric form of P18 in the solution phase. The individual particles of the probe in the aggregated form were distinctly observed in a rectangular shape. FESEM images exhibit a large number of aggregated islands of the monomeric P18 particles in the solid state. Interestingly, the P18 particles in each of the aggregated islands get agglomerated with each other in a solid state. Close inspection on the nature of agglomeration suggests that most of the individual particles participated in fusion with others using different edges of the rectangular-shaped particle. It is better to say that a head-totail type of interlocking of individual particles was observed through the linking of rectangular particles' edges in the aggregated form. The average size of the individual particles was determined as ~ 250(±3) nm from the FESEM images. Furthermore, EDX spectral characterisation with elemental mapping is used to determine the elemental distribution in the formation of aggregate. EDX spectrum (Fig. 1b) shows a %elemental distribution of C and N to the aggregated form. Elemental mapping for P18 (Fig. 1c) further consolidates the observation noticed in EDX plot of the nanoaggregates. Moreover, the size of the aggregated form of P18 was determined with dynamic light scattering (DLS) measurements (Fig. 2). The DLS plot of P18 in the aqueous phase indicates that the average particle size of the aggregated form is $270(\pm 3)$ nm. The effect of the solution concentration on the aggregation behaviour of P18 was also examined. The particle size increased with

the increase of the concentration of monomeric P18 in the solution phase.

3.4. Spectroscopic studies on the P18 aggregate

The insight of the molecular aggregation and the nanoaggregates' photophysical properties were investigated in detail. Fig. S5 showed the comparison of the spectral bands of P18 and its aggregated form, respectively. It is well observed from Fig. S5 that the absorption spectral profile of P18 aggregates (272 and 306 nm) is red-shifted compared to the monomeric form of P18 (263 and 285 nm) in the aqueous phase. Literature on molecular aggregation suggests that a red-shift of the electronic band for a species commonly happens for the J type of aggregation [17,18]. In this case, an average red-shift of ~ 10–20 nm was noticed for the absorption bands of the P18 aggregates compared to its monomeric form, and this phenomenon is a pure indication for the development of J aggregates in the aqueous phase.

To consolidate the origin of the red-shift in the aggregated form of P18 and find out the solvent role, the polarity of the solvent was varied. The absorbance of P18 was measured in another polar system (methanol:water), where the polarity of the solvent mixture was kept close to that of water:DMSO solvent mixture. The absorption maxima of P18 in the methanol:water mixture found at 261 nm that was lower than the wavelength maximum (272 nm) of P18 aggregates. The larger red-shift of the electronic band for P18 nano-aggregates confirms that the solvent polarity didn't induce this red-shift of the electronic band; perhaps the structural aggregation remains the driving force for the P18 aggregation. The molecular exciton theory may explain the shifts in the electronic band of the aggregated forms [44]. By the principle of molecular exciton theory, a molecule is treated as a point dipole, and the excitonic energy state of the molecular aggregate may be split into two tiers based on the nature of dipoles [45]. The resultant electronic transition may proceed through lower or higher energy transitions leading to J and H type of molecular aggregation. The different kinds of dipole-dipole interactions within two monomers in the aggregated form are principally accountable for splitting energy levels in the molecular aggregates [45].

The molecular exciton theory further suggests that face-to-face interactions of the transition dipoles for H-aggregates make a shift of absorption maximum towards the blue region while a head-totail type of orientations for J-aggregates makes a shift in absorption maximum to the red region. Crystal structure analysis and detailed study on self-assembly of P18 provide an essential source of light on this aspect. The excited states of these aggregates are also investigated with the measurement of steady-state and time-resolved fluorescence studies. Fig. S6 displays the comparison of the



Fig. 1. a) FESEM images for the aggregate form of P18; b) Elemental mapping of the molecular aggregate of P18; c) EDX plot showing the distributed % of C and N in the aggregated form.



Fig. 2. Dynamic light scattering measurement of P18 in the aggregated form in aqueous médium.

fluorescence spectra of P18 in its monomeric with the aggregated forms under identical parameter set up.

It is evident from Fig. S5 that upon excitation on 272 nm, the emission maxima for the P18 nano-aggregate was red-shifted than

its monomeric form. The fluorescence intensity of the P18 nanoaggregate enhanced by ~ 20 fold in intensity with the emission of blue light. Therefore, upon aggregation, the mildly fluorescent monomeric P18 turns out to be highly fluorescent with blue light



Fig. 3. Time-dependent photoluminescence decay profile for P18 in aggregated form.

emission. The measurement of an average lifetime in the aqueous phase, estimated as t = 0.99 ns (Fig. 3) further confirmed the highly emissive characteristics of the nano-aggregate. The excited states of the nano-aggregate get stabilised upon interlocking of the aromatic rings for P18 in the aqueous medium and exhibit intense blue light emission.

3.5. Description of crystal structure and self-assembly

The single crystals of P18 were successfully grown in solution to reveal the nature of weak intermolecular forces in the development of nano-aggregate. The crystal structure analysis revealed that the molecule crystallised in a monoclinic crystal system. The ball and stick model of the asymmetric unit and molecular structure of the Schiff base is shown in Fig. 4a and Fig. 4b. The structural refinement parameter is summarised in Table 1. The bond distances and bond angles of the compound are presented in Table S1. The Schiff base crystallised in a nearly planar *antistereomer* as revealed by the bond angles' measurement (Fig. 4d, Table S1). The C6-N2 and N2–N2a bonds correspond to a pure double and single bond character, as evident from their bond distance values, 1.295(±0.0017) Å and 1.3888 (±0.0015) Å, respectively (Tables S1).

The packing diagram of the Schiff base showed edge to face type orientations of the asymmetric units along the *b* axis (Fig. S7). There is no considerable intermolecular H-bonding in the self-assembled structure. However, long distant $\pi...\pi$ and short-ranged C–H... π interactions play a significant role in forming self-assembled crystalline architecture. Interaction mapping over the molecule further suggests the high propensity of the hydrophobic interaction (Fig. 4C). In the structure of P18, four aromatic rings (two pyridine and two phenyl rings) are connected to imine-Cs through N–N single bonds in this molecule. Close inspection on the supramolecular framework (Fig. 5) suggests that the pyridine centroids stacked through a weaker $\pi...\pi$ interactions, while the



Structural refinement parameter of the Schiff base.

Parameters	P18
Empirical formula	C24H18N4
Formula weight	362.42
Temperature (K)	100
Crystal system	Monoclinic
Space group	C2/c
a (Å)	21.6921(9)
b (Å)	5.5760(2)
c (Å)	15.2461(5)
Volume (Å3)	1840.79(12)
Z	4
ρ (gcm-3)	1.308
μ (mm–1)	0.079
F (000)	760
θ ranges (°)	2.7-32.8
R(int)	0.030
Number of unique reflections	3208
Total number of reflections	10,872
Final R indices	0.0668, 0.2199
Largest peak and hole (eA-3)	0.58, -0.50

phenyl centroids exhibited short-ranged C–H··· π interactions in the crystalline phase (Table S2) [46,47].

3.6. Hirshfeld surface and energy framework analysis

The Hirshfeld surface analysis was further carried out to understand the role of intermolecular interactions, as illustrated in Figure S8. The surface volume and surface area of P18 were calculated as 451.84 Å³ and 411.11 Å², with asphericity and globularity indices evaluated as 0.094 and 0.693, respectively. The intermolecular interactions of P18 are also manifested in terms of two dimensional fingerprint plots between d_e and d_i (Fig. S9). The highly influential C–H··· π interaction contributes nearly 31.5% of total Hirshfeld surface coverage having a nearly sharp



Fig. 4. Displacement ellipsoid representation of the molecule: (a) Asymmetric unit of the Schiff base; (b) Ball and stick model of the compound; (c) Interaction propensity of the molecule; (d) Planarity of the asymmetric unit.



Fig. 5. Development of long-range crystalline architecture of P18 mediated by C-H $\cdots\pi$ and π $\cdots\pi$ interactions.

tooth in fingerprint plots which indicates the strength of interaction. The π ... π interaction has only about 3% of Hirshfeld surface coverage, and the bright blue spot on fingerprint plot represents the strength of the interaction. The absence of any sharp tooth from fingerprint plots indicates the lack of any strong hydrogen bonding interactions in the molecule, i.e. less contribution from the Coulumb energy parameter in total energy expression. One centroid of an electron-deficient pyridyl moiety attracts two C – H protons of electron-dense benzene ring forming C–H(dono r)... π (acceptor) interaction where electron density of electrondeficient pyridyl moiety is increased to some extent over the other electron-deficient pyridyl ring (oriented in head-to-tail fashion) which bears a single C–H(donor) $\dots \pi$ (acceptor) interaction. The C– H... π and π ... π interactions are the only interactions involved in developing long-range supramolecular crystal architecture. The percentage share of individual elements with other elements for crystalline architecture is presented in Table S3.

The energy framework analysis is computed on Crystal Explorer 21.2 software (Turner et al., 2017, Mackenzie et al., 2017) with HF/3-21G basis sets using TONTO software for the cluster environment of 3.8 Å surrounding a particular molecule of interest. The total interaction energy is articulated as $E_{tot} = k_{ele}$ - $\dot{E}_{ele} + k_{pol}\dot{E}_{pol} + k_{disp}\dot{E}_{disp} + k_{rep}\dot{E}_{rep}$, where the k values belong to the scale factors for benchmarked energy models. \dot{E}_{ele} represents the electrostatic energy, E_{pol} represents the polarisation energy, \acute{E}_{disp} represents the dispersion energy, and \acute{E}_{rep} represents the repulsive energy (Table S4). To identify the type of interaction energies developed due to supramolecular interactions, we set the tube dimension factor 300 where a greater tube radius is directly proportional with stronger and more prominent interaction. From Fig. 6 it is clearly evident that the contribution of dispersive forces in total interaction energy is maximum over coulomb energy. These short-ranged dispersive forces account for isoenergetic and isotropic C–H··· π and π ··· π interactions, thus playing a



Fig. 6. (a) Energy framework diagram, (b) total energy plot, (c) coulomb energy contribution plot, and (d) dispersive energy contribution plot mapped for P18 along b-axis.

significant role in aggregation behaviour of P18. The predominance of dispersive forces is justified by the greater inner dimension of green cylinders than red cylinders between the same molecules. The total dispersive energy involved in the cluster of molecules is estimated to be -192.4 kJ/mol.

3.7. Structural perspectives and underlying mechanism for AIE property of the Schiff base

To decipher the role of weak forces for the assembled polarised or non-polarised aromatic molecules in supramolecular organic frameworks, we explored the propensity of dispersive energy for intermolecular C–H··· π and π ··· π interactions in the clusterisation of P18. Interesting, Martinez et al. [48] attributed a valuable insight for the driving force in the association of polarised/non-polarised aromatic molecules through different proposals based on experimental observations and theoretical calculations such as the polar/ π model [49], alternating e-rich and e-deficient aromatic- π interactions [50,51], propensity of heteroaromatic π -systems [52] and a large contact surface of π -electrons [53]. The synthetic Schiff base contains flat and robust type phenyl and pyridine rings with a relatively large contact surface that might enable the dispersion force-induced stabilisation of the molecular aggregate as proposed by Martinez et al. [52]. However, flexible conformation with twisted orientations of aromatic rings facilitates the steric hindrance among the neighbouring aromatic rings, leading to a long distant face-to-face aromatic interaction [54]. It is scientifically evident that considerable intermolecular C–H... π interactions, also known as edge-to-face [55]. T-shaped [56], can stabilise the crystal packing through restricted rotational orientations of the aromatic rings and make a pronounced effect on the molecular properties. Nishio and co-workers envisioned a significant effort to obtain valuable insights into the nature of C–H… π interactions [21,57]. They reported that orientations of aromatic rings causing C–H $\cdots\pi$ interactions have a significant contribution in molecular packing and self-assembly.

It is a well-established fact that the charge transfer of π -e to the anti-bonding orbital of C–H bond principally account for the origin of C–H··· π interactions [58,59]. Nishio et al., surveyed the C–H··· π interactions for 6-membered π -electronic systems varying the positions of hydrogen atoms on a π -plane [57] (Scheme 2), where D_{pln} , D_{lin} and D_{atm} define the H··· π (plane), H···(C₁C₂ line) and H···C₁ distances, respectively. The dihedral angles between the π -plane and HC₁C₂ plane as \angle HXC₁ angle (X = C,O, etc.) are represented as ω and θ , respectively. This model was applied by considering H··· π distances shorter than a cut-off D_{max} value and $D_{\text{pln}} < D_{\text{max}}$, $\theta < 60^\circ$, $|\omega| < 90^\circ$ for region 1; $D_{\text{lin}} < D_{\text{max}}$, $\theta < 60^\circ$, $90^\circ < |\omega| < 130^\circ$ for region 2; $D_{\text{atm}} < D_{\text{max}}$, $\theta < 60^\circ$, $50^\circ < \phi < 90^\circ$ for region 3 (ϕ = HC₁I).

This method is advantageous to validate the C–H···Ar contacts, and it is revealed that higher acidic-H will give rise to shorter mean values of H··· π distances and the D_{pln} , and D_{atm} will also produce smaller values. They obtained the mean H... π distance for aromatic- C–H··· π aromatic interaction as 2.76 ± 0.10 Å for a 32,282 number of CH···Ar contacts [57]. Previously, Alvarez reported an interesting work for intermolecular contacts showing



Scheme 2. C-H... π surveying model; a) O is the centre of the plane, C₁ and C₂ nearest and second nearest sp²-C to H, ω is the dihedral angle, \angle C₁OC₂ and \angle HC₁C₂, θ is \angle HXC₁; b) Region: Reg1, H is above on π -aromatic, Reg2 and Reg3 indicates H is out of the aromatic ring but may interact with π -electrons.

distance distribution maps between an element and a probe element, X, mostly oxygen [60]. The author summarised that most elements reserve a different distance in the distribution and provide a clear depiction between bonded and non-bonded atom pairs [60]. We also attempted to validate and examine the propensity of C–H··· π interactions for P18 and tetraphenylethene (TPE) following the method of Nishio et al. The measurement of D_{pln} , D_{lin} , θ and ω was well corroborated between P18 and TPE (Table S5).

Furthermore, the underlying principle of the AIE properties for this Schiff base was unveiled by comparing the structural characteristics of a widely studied tetraphenylethene (TPE) which exhibited a pronounced AIE phenomenon with the synthetic P18. TPE is a nearly planar non-emissive molecule (Fig. S10) in solution because the excited-state energy of TPE dissipates through the free-rotations of the four phenyl rings attached to ethylene-C [2.61.62]. However, intermolecular interactions restrict the intramolecular movement of the phenyl rings in the aggregated state and enable them to emit bright light [2,61,62]. It is well established that TPE locked the phenyl rings in aggregated form based on restriction of intramolecular rotation (RIR) and vibrations (RIV), leading to an intriguing turn-on of fluorescence properties in molecular aggregates [61,62]. The X-ray crystal structure of TPE was previously reported by Hoekstra et al. [63], and we downloaded the deposited CIF from Cambridge Structural Database (CCDC 1275289) to compare structural features and C–H $\dots\pi$ contribution in the construction of supramolecular frameworks. Fig. S10 (a,b,c,d) displayed a combination of crystal structure, structure with selected bond distances and angles and interaction mapping of TPE which displayed close structural characteristics of P18. Further, TPE showed two different short-ranged C–H $\dots\pi$ interactions (2.76 Å & 2.91 Å) while P18 showed one short C–H… π interactions (2.94 Å) with one distant (3.18 Å) C–H \cdots π interactions (Fig. S11). Both the compounds exist in nearly planar structures and exhibited a similar propensity for hydrophobic interactions (Fig. S10-b, c,d).

We also considered a previously reported azine compound, salicylaldehyde azine (SAA), comparing AIE properties with P18, Typically. SAA adopts complete planarity due to its strong intramolecular hydrogen bonding interaction; however, the complete planarity of P18 molecule cannot be achieved without any intramolecular H-bonding. SAA exhibits excited-state intramolecular proton transfer (ESIPT) and AIE characteristics [64,65]. AIE and ESIPT processes are entirely different, although both are mutually compatible to turn on the fluorescence property of the molecules. The AIE property stems from RIR and RIM characteristics leading to emission enhancement, while ESIPT facilitated by excited-state proton transfer and consequent causing of significant Stokes shift with bright emission. In contrast to SAA, the synthetic P18 molecule displayed predominance short C–H··· π interactions. Therefore, based on a spectroscopic, photophysical and detailed study on selfassembly, energy framework analysis, it is recommended that interlocking of head-to-tail type of aromatic rings through dominant C-H··· π short contacts lead to the nano-dimension aggregation with intense blue light emission.

4. Conclusions

Herein, we studied the aggregation characteristics of a newly designed azine type Schiff base with a suite of spectroscopic, photophysical, and crystallographic methods. The nearly planar structure of the probe was established with single crystal X-ray diffraction analysis and different spectroscopic methods. Interesting, supramolecular frameworks of the compound adopted long distant π ... π interactions and short C-H··· π interactions (>2.92 Å) beyond vdW limit without considerable intermolecular

hydrogen bonding in crystalline phase. Hirshfeld surface analysis suggests that highly influential C–H $\dots\pi$ interaction contributed nearly 31.5% while long-distant $\pi \cdots \pi$ interactions have only about 3% of total Hirshfeld surface coverage. The total dispersive energy involved in the cluster of molecules is manifested in terms of C-H... π interactions and estimated to be -192.4 kJ/mol to the stabilisation of aggregate. The nano-cluster of the probe in the aggregated form displayed the development of intensively emissive blue light. The beautiful rectangular-shaped particles of an average hydrodynamic size of 270(±3) nm propagate through the head-totail type interlocking of aromatic rings mediated with short C–H $\cdots\pi$ and long $\pi \cdots \pi$ interactions enables a restriction to the intramolecular motion of the probe leading to nano-clusters in the solid state. Therefore, exploitation of spectroscopic, photophysical and crystal engineering perspectives on this molecular aggregation phenomenon will undoubtedly throw some new structural insights to understand the role of intermolecular interactions (specially C–H··· π associations) for the formation of molecular aggregates. We deeply believe that suitable adaptation of the azine chromophore of this molecule may envision new supramolecular organic frameworks (SOF) with intriguing AIE properties and may act as a probe of great promise for designing optoelectronic devices and green energy harvesting phenomenon.

CRediT authorship contribution statement

Prafullya Kumar Mudi: Conceptualization, Formal analysis, Methodology, Investigation. **Ajit Das:** Formal analysis, Methodology, Investigation. **Nagendranath Mahata:** Formal analysis, Visualization. **Bhaskar Biswas:** Conceptualization, Writing – review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.molliq.2021.117193.

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