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Article

A Low Temperature Fluorescence Study of a 4-Dimethylamino-2′-Hydroxy Chalcone: From Solvent Matrix to Crystalline State

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Abstract

4-Dimethylamino-2′-hydroxy chalcone (DHC) **1** is an important natural compound that is nearly non-fluorescent in solution but highly fluorescent in its crystalline state. At room temperature, the weak fluorescence from DHC solution is exclusively from its *keto* tautomer, without notable contribution from its *enol* tautomer. By using low temperature fluorescence, the study found that the *enol* emission could be detected upon cooling with liquid N_2 in a protic solvent (e.g. EtOH). This led to observation of the fluorescence vibronic structure of *enol* tautomer, in addition to its *enol* emission $\lambda_{em} \approx 473$ nm that is well separated from its *keto* tautomer emission ($\lambda_{em} \approx 600$ nm). By freezing DHC in a solvent matrix, the study revealed the fluorescent characteristics of a single molecule in a rigid environment. Further comparison of DHC in a solvent matrix and crystalline state disclosed that the emission of crystalline DHC was primarily from the *keto* tautomer, along with some minor contribution from the *enol* tautomer, despite the tight packing environment in the crystalline state.

Keywords: fluorescence; UV–vis spectroscopy; low-temperature fluorescence; synchronous fluorescence; excited-state intramolecular proton transfer (ESIPT); 2′-hydroxychalcone

1. Introduction

Chalcones are a group of organic compounds widely distributed in plant metabolic systems.[1] General structure of chalcones consists of two aromatic rings that are connected by an α,β-unsaturated carbonyl unit, a motif that provides extensive π-conjugation. As a result, this class of compounds often exhibit low toxicity and attractive optical properties. Among them, 2′-hydroxychalcone derivatives are especially of interest,[2,3, 4] as their structure contains an intramolecular O–H···O=C hydrogen bond, which can undergo excited-state intramolecular proton transfer (ESIPT), giving rise to large Stokes shifts and red-shifted emission. For example, 2′-hydroxychalcone DHC **1** (Scheme 1) is known to give emission with a large Stokes' shift (e.g., $\lambda_{abs} \approx$ 430 nm, $\lambda_{em} \approx 620$ nm in benzene, and $\Phi_{fl} \approx 4.6 \times 10^{-6}$).[3] Despite its low fluorescence in solutions, **1** exhibits remarkably high fluorescence quantum yield in crystalline state (Φ_{fl} =0.32), which is among the highest for reported organic crystals.[2] In addition, the crystals of **1** also give near infrared (NIR) emission at about 710 nm. The striking enhancement has enabled the use of **1** for various fluorescent sensors, including detection of biothiols,[5] alkaline phosphatase activity in live cells,[6] latent fingerprint[7] and cellular Al^{3+} ion that is associated with Alzheimer's disease.[8] In the sensor design, ESIPT is often coupled with aggregation-induced emission (AIE) to improve signal contrast.

In solution, DHC **1** could exist in either *enol* or *keto* forms upon photoexcitation. By using ultrafast spectroscopy, previous studies from Abou-Zied et al.[9] has shown that the initially excited *enol* form of **1** (MeOH solution) quickly undergoes tautomerization (in ~3 picoseconds) to form the *keto* tautomer that is stable in its excited state. The steady state fluorescence detected only one weak emission peak at ~575 nm ($\Phi_{fl} < 0.01$) that is attributed to the *keto* tautomer. In addition to ESIPT, intramolecular torsional motion between the A-ring and the C=O group (Scheme 1) has been

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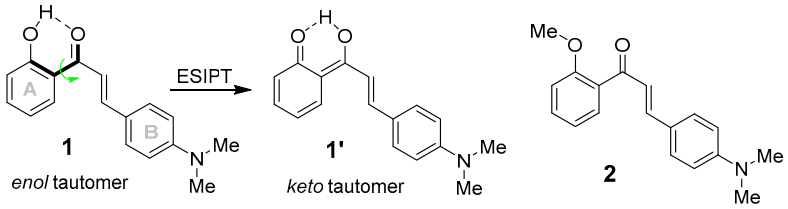
identified as an efficient nonradiative decay pathway that further suppresses fluorescence in solution.[4]

A fundamental question is why chalcone **1** exhibits dramatically enhanced and red-shifted emission in the solid state despite its weak fluorescence in solutions. A possible reason for observing high fluorescence from solid state **1** is that the chalcone molecules become more rigid due to the packing in the solid state, which reduces the molecular rotation and vibration. However, solid-state packing will also bring chalcone molecules into close contact, which could induce aggregate and excimer formation, thus affecting its fluorescence. In order to shed additional light on the intrinsic molecular fluorescence without significant intermolecular interaction, we decided to examine its low temperature fluorescence in dilute solution. In the experiment, an individual molecule would be well separated from the others by freezing **1** in a solvent matrix. Thus, the tautomerization of *enol* to *keto* form would be associated with the intrinsic molecular property, without being affected by solid-state packing. Herein we report the low temperature fluorescence of **1**.



Scheme 1. Chemical structure of 2-hydroxy chalcone (DHC) **1** and its derivative **2**.

2. Materials and Methods

Chalcones **1** and **2** were synthesized by using the literature procedure.[10] To a stirring solution of the corresponding acetophenone (5 mmol) and benzaldehyde (5.5 mmol) in EtOH (15mL) was added potassium hydroxide (15mmol). The mixture was stirred at room temperature overnight. The crude product was collected via filtration followed by recrystallization in EtOH to yield the pure product as a red crystalline solid (**1**) and an orange solid (**2**). ^{1}H NMR spectra (ESI Figures S1 and S2) were compared with literature reports and found to be consistent.

^{1}H NMR spectra were obtained on a Varian 300 MHz spectrometer. UV-Vis spectra were acquired by using a Hewlett Packard-8453 diode array spectrophotometer at 25 ^{0}C. Fluorescence spectra were measured by using a HORIBA Fluoromax-4 spectrofluorometer.

3. Results and Discussion

Chalcone **1** was synthesized according to reported procedures, and full characterization data are provided in the supporting information. In order to aid the spectral characterization, we also synthesized compound **2** (by using a literature procedure),[11] in which the hydroxy group was replaced with a methoxy group to eliminate the excited state intramolecular proton transfer (ESIPT) process.

At room temperature, UV–Vis absorption of **1** revealed a peak at λ_{max} = 433 nm in EtOH (Figure 1a). The excitation spectrum of **1** in EtOH also revealed a broad maximum at 445 nm (Figure 1b), in consistency with the observed absorption spectrum. The fluorescence spectrum of **1** displayed a broad weak emission peak ($\lambda_{em} \approx$ 590 nm) with a large Stokes shift (≈ 5,520 cm^{-1}), which is typical of ESIPT fluorophores and is attributed to *keto* emission following ultrafast ESIPT.

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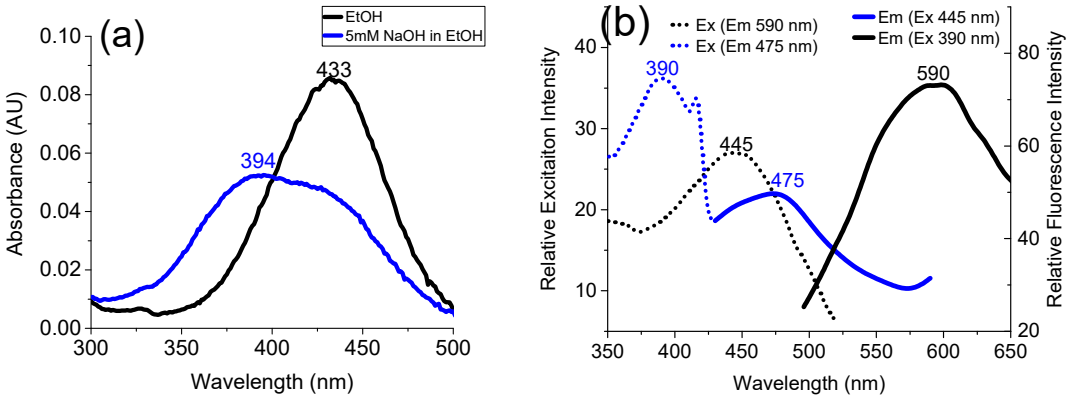

Figure 1. UV-vis absorption spectra (a) and fluorescence excitation (dotted line) and emission spectra (solid line) (b) of DHC **1** (2.5 μM) in EtOH (black curve) and 5 mM NaOH in EtOH (blue curve) at room temperature.

The spectral studies of **1** indicated possible presence of multiple emissive species in solution at room temperature (Figure 1). In order to gain further information about the emissive species, fluorescence measurements were performed at 77 K in ethanol. Rapid cooling of the ethanol solution would trap an individual molecule of **1** in a rigid solvent matrix at 77 K, thereby leading to significant spectral narrowing by suppression of thermally accessible bond rotations and vibrational broadening. Interestingly, the low temperature spectra revealed structured emission, showing emission bands at 580, 600, and 648 nm, when excited at 472 & 480 nm (Figure 2b). By monitoring the emission at 580, 600 and 648 nm, the excitation spectra revealed the same profile, implying that these emission bands originated from the same species (i.e. *keto* emission). Interestingly, an additional higher-energy emission band was observed near 467 nm, when excited at 430 and 450 nm (Figure 2b). The results suggested the presence of an additional neutral emissive species, which could be attributed to the *enol* tautomer.

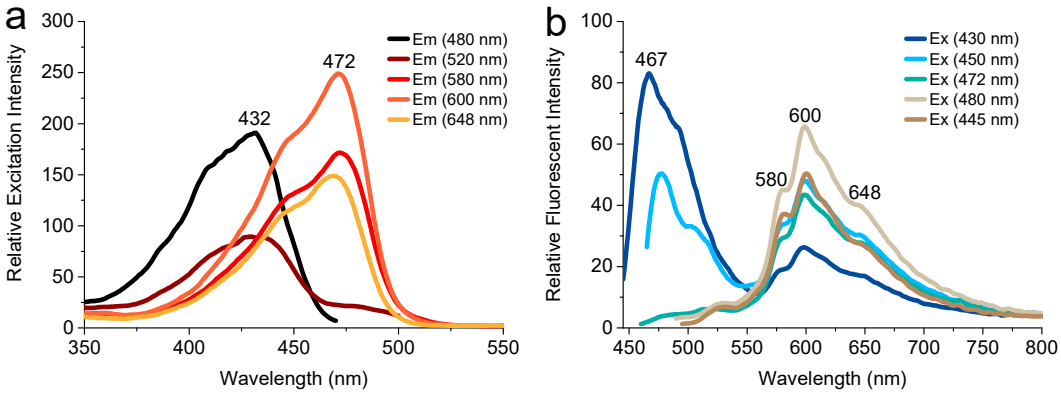

Figure 2. Excitation spectra (a) monitored at selected emission wavelengths and emission spectra (b) recorded at selected excitation wavelengths for **1** (2.5 μM) in EtOH at 77 K.

In order to further verify that emission of **1** at 467 nm in EtOH at 77 K (Figure 2b) originates from the *enol* tautomer, low-temperature measurements were performed in ethanol containing 5 mM NaOH (Figure 3). Under basic conditions, both excited *enol* and *keto* forms will become one species (i.e. phenoxide Ar-O⁻), whose emission would be similar to *enol* (without undergoing ESIPT). At room temperature, the phenoxide exhibited a broad blue-shifted absorption ($\lambda_{max} \approx 394$ nm) and emission ($\lambda_{em} \approx 475$ nm) (Figure 1). At 77 K, the frozen anion of **1** in EtOH exhibited a structured emission (λ_{em}

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≈ 482, 512 & 550 nm) (Figure 3b), which was comparable to that of the *enol* emission of neutral **1** in EtOH (λ_{em} ≈ 467 & 489 nm, Figure 2b). This assignment was further supported by an acid-recovery control, in which the phenoxide of **1** was acidified with HCl at room temperature ($Ar\text{-}O^- + H^+ \rightarrow Ar\text{-}OH$) prior to freezing, thus reenabling the ESIPT process (ESI Figure S5).

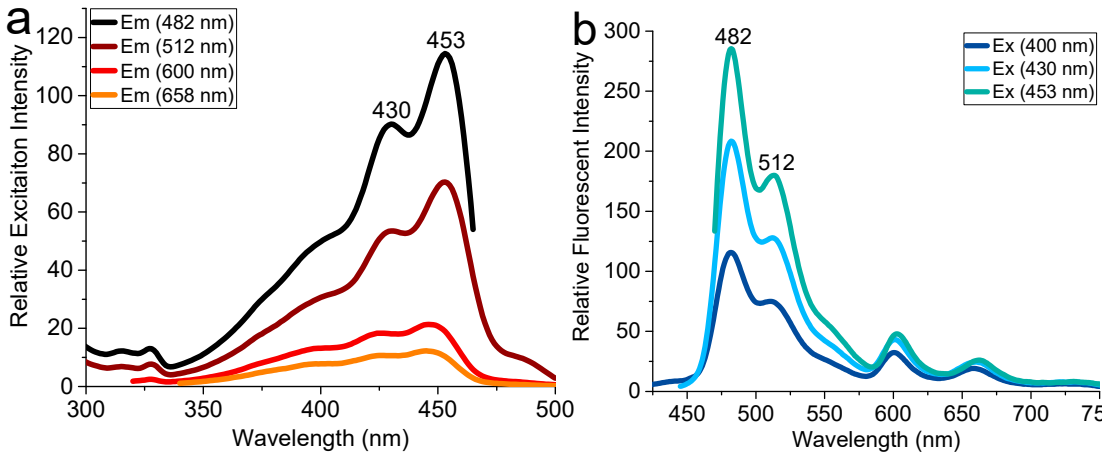

Figure 3. Excitation spectra (a) monitored at selected emission wavelengths and emission spectra (b) recorded at selected excitation wavelengths for **1** (2.5 μM) in 5 mM NaOH/EtOH at 77 K.

Synchronous fluorescence scan was used to further distinguish the *enol* from *keto* emission in the frozen **1** (Figure 4). As shown from Figure 2, the *enol* emission of **1** (λ_{em} ≈ 467 nm) was separated from its excitation (λ_{ex} ≈ 432 nm) by $\Delta\lambda$ ≈ 35 nm, while its *keto* emission was separated by $\Delta\lambda$ ≈ 128 nm (=600–472 nm). In EtOH at 77 K, when $\Delta\lambda$ was near 35 nm, it selectively enhanced the *enol* emission at 467 nm (Figure 4). While $\Delta\lambda$ ≈ 128 nm, the spectrum selectively enhanced the *keto* emission in the 580–650 nm regions. The observed distinct effect of Stokes shifts on the emission profiles thus presented additional evidence for the presence of both *enol* and *keto* emissions of **1**. The *keto* emission was not detected when **1** was in 5 mM NaOH/EtOH at 77 K (ESI Figure S6).

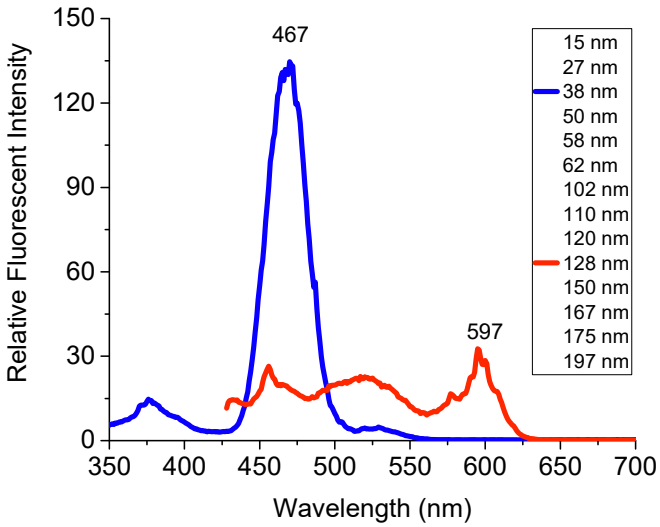

Figure 4. Synchronous fluorescence spectra of chalcone **1** (2.5 μM) at 77 K in EtOH acquired at variable wavelength offsets ($\Delta\lambda$ = 15–197 nm).

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As shown in Figure 2b, the *enol* and *keto* emissions are *co*-existent, due to efficient ESIPT process in **1**. In order to completely eliminate ESIPT contribution, chalcone **2** was selected as a control in which the 2′-hydroxy is replaced with a methoxy group, which disables ESIPT and proton-dependent photophysical processes. This modification preserves the conjugated chalcone framework while removing the structural feature responsible for proton-dependent photophysical contributions in **1** (such as the acid–base behavior), which complicates evaluation of intrinsic properties of the chromophore. At room temperature, the EtOH solution of **2** gave an absorption λ_{max} = 405 nm and emission λ_{em} = 550 nm. No noticeable spectral shifts were observed upon addition of base or acid (ESI Figure S7 and S8). Additionally, synchronous fluorescence measurements of **2** in ethanol and basic ethanol showed a uniform emission profile with a maximum at $\Delta\lambda \approx 145$ nm (Figure S9), consistent with one dominant emissive species in solution.

The photophysical properties of **2** were further examined at 77 K in ethanol (Figure 5), which revealed more structured well-resolved bands at 456, 488, and 522 nm with approximately regular spacing in wavenumber (~1300–1450 cm^{-1}). The observation indicated vibronic structures arising from a single emissive state (not emission from multiple species). It should be noticed that the emission at the low temperature was likely from a locally excited state, as bond rotation and vibration were inhibited in a frozen matrix. Similar conjugation length between **1** and **2** could be illustrated by their similar low temperature emission wavelengths, i.e. $\lambda_{em} \approx 456$ & 488 nm for **2** (Figure 5) and $\lambda_{em} \approx 467$ nm for **1** (Figure 2b). It was also noticed that the fluorescence at $\lambda_{em} \approx 488$ nm was significantly hypochromically shift from its $\lambda_{em} \approx 550$ nm at room temperature. At the room temperature, intramolecular charge transfer (ICT) can occur between a donor (-NMe_2) and acceptor (C=O) group, giving a long wavelength emission. This ICT interaction could be disabled in the low temperature, as the associated bond alternation and vibration is inhibited.

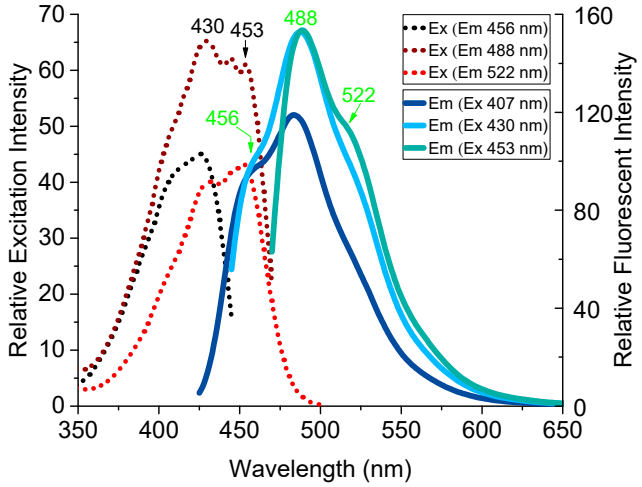

Figure 5. Excitation spectra (dotted lines) monitored at selected emission wavelengths and emission spectra (solid lines) recorded at selected excitation wavelengths for **2** (2.5 μM) in EtOH at 77 K.

To probe the role of intermolecular interactions, a solid film of **1** was prepared by slow evaporation of a methylene chloride solution onto the inner surface of a quartz tube at room temperature. At room temperature, the film exhibited a strong fluorescence band centered at ~660 nm (inset in Figure 6), consistent with the reported emission of crystalline **1**.[9,12] When the same sample was cooled with liquid N_2 to 77K, the spectrum appeared to be broader, showing an additional higher-energy emission as a shoulder at ~612 nm alongside the dominant ~660 nm band (Figure 6). To better explain the result, the fluorescence spectrum at 77K was fitted with Gaussian functions that deconvolute the spectrum into two peaks at 610 and 660 nm. The major peak at 660 nm could be attributed to the ESIPT-derived *keto* emission in the solid state.

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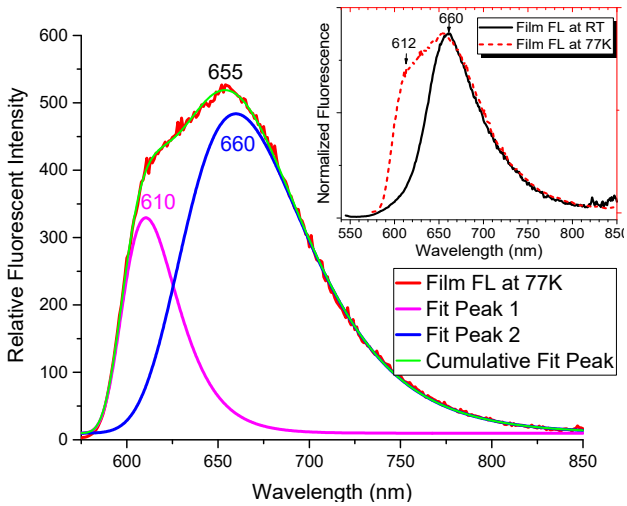

Figure 6. Fluorescence spectra of film **1** at 77K, along with two deconvoluted bands. The inset shows the normalized fluorescence at room temperature and 77K.

Observation of the minor peak at ~612 nm at low temperature, which was absent at room temperature, indicated interruption of excited-state relaxation pathways that dominate at room temperature. The aggregation was not likely the reason, as aggregate formation could not explain why only a small fraction of molecules in the solid was affected. The possibilities of suppressing ICT could be ruled out, since ICT is expected to be disabled at the low temperature.[13] This led us to assume that the minor emission peak could be associated with the incomplete proton transfer in the crystalline solid. It was noted that a smaller spectral shift of $\Delta\lambda \approx 48$ nm (=660–612 nm) was observed in a tightly packed crystalline state (in comparison with the frozen amorphous solvent matrix). In addition to the packing, the local polarity environment could also affect the spectral shift between the *enol* and *keto* emissions.

4. Conclusions

Low-temperature fluorescence has been used to study the photophysical property of 2′-hydroxychalcone **1**. Under ambient temperature, the fluorescence of **1** displays only *keto* emission in both protic (e.g. EtOH) and aprotic (e.g. hexane) solvents. The difficulty to observe the *enol* emission of **1** can be attributed to its very low fluorescence and ultrafast ESIPT. By using liquid N_2 to freeze the molecular **1** in a solvent matrix at 77K, this study demonstrates that both *enol* and *keto* emissions can be observed directly in a protic solvent (i.e. EtOH). The study thus illustrates the effect of intermolecular H-bonding on the ESIPT process of **1**. It should be noted that solvent effect on *enol/keto* tautomer ratio had been reported from a structurally related 3-hydroxyflavone at room temperature, which exhibits exclusive *keto* emission in alkanes but significant *enol* emission in EtOH.[14] The required low temperature to detect *enol* emission in a protic solvent suggested that the ESIPT process in **1** could be faster than that in 3-hydroxyflavone.

As shown in Scheme 2 below, intermolecular hydrogen bonding between the phenolic hydroxyl group and surrounding ethanol molecules competes with the intramolecular O–H···O=C hydrogen bond required for ESIPT. It was assumed that majority of chalcone **1** would exist in the solvate form, as illustrated in a reported study from a structurally similar 3-hydroxyflavone.[15] The content of "solvated 1" could be increased at the low temperature. The assumption is supported by Gibbs Free Energy equation $\Delta G° = \Delta H° - T\Delta S°$, which predicts that the entropy-related effects will be kept at a minimum level at the low temperature. The increased content of "solvated **1**", in combination with increased molecular rigidity, facilitated the detection of its *enol* tautomer of **1**.

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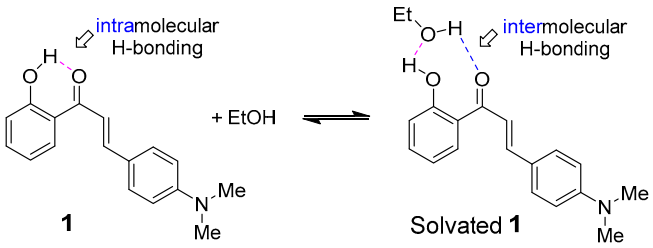

Scheme 2. Schematic illustration of solvation of **1** with EtOH.

The spectral feature of the *enol* emission has been further confirmed through comparison with the methoxy-substituted derivative **2**. The study thus successfully identified the *enol* emission of **1** that is well separated from its *keto* emission (by >130 nm, Figure 2). Byisolating individual molecular **1** in a rigid EtOH matrix, structured emission from both *enol* and *keto* tautomer can be observed without interfering from chromophore-chromophore interaction.

Extending the low temperature fluorescence study to a solid film reveals that a dominate emission from the *keto* tautomer (λ_{em} ≈660 nm) , which is accompanied with a minor emission (λ_{em} ≈610 nm). Based on the spectral blue shift, the minor emission could be related to *enol* emission, which might occur on the surface of the solid film.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/doi/s1, Figure S1: ^{1}H NMR of 1 (300MHz, CDCl3) δ 13.16 (s, 1H, OH), 7.94-7.91 (s, 1H), 7.94-7.89 (d, J = 15.22 Hz, 1H), 7.58-7.55 (d, J = 9.08 Hz, 2H), 7.48-7.43 (t, J = 7.49 Hz, 1H), 7.47-7.42 (d, J = 15.22 Hz, 1H), 7.02-6.99 (d, J = 8.20 Hz, 1H), 6.95-6.89 (t, J = 7.49 Hz, 1H), 6.70-6.67, (d, J = 9.08 Hz, 2H), 3.05 (s, 6H, NMe2); Figure S2: ^{1}H NMR of 2 (300MHz, CDCl3) δ 7.57-7.55 (d, J = 8.20 Hz, 1H), 7.57-7.52 (d, J = 15.81 Hz, 1H), 7.49-7.46 (d, J = 8.78 Hz, 2H), 7.46-7.41 (t, J = 7.61 Hz, 1H), 7.15-7.10 (d, J = 15.81 Hz, 1H), 7.05-7.00 (t, J = 7.61 Hz, 1H), 7.00-6.97 (d, J = 8.20 Hz, 1H), 6.68-6.65 (d, J = 8.78 Hz, 2H), 3.87 (s, 3H, OMe), 3.02 (s, 6H, NMe2); Figure S3: Absorbance (dotted lines) and fluorescence (solid lines) spectra of chalcone 1 (2.5 μM) in 5 mM NaOH/EtOH. The sharp emission at 449 nm in the emission spectra is attributed to Raman ethanol scattering due to low fluorescence; Figure S4: Excitation (gray) spectrum monitored at 482 nm and emission (black) spectrum recorded at λex = 453 nm for 1 (2.5 μM) in 5 mM NaOH/EtOH at 77 K; Figure S5: Excitation (dotted) and emission (solid) spectra of 1 (2.5 μM) in 5 mM NaOH/EtOH after acidification with 1 equivalent HCl at 77 K; Figure S6: Synchronous fluorescence spectra of chalcone 1 in 5 mM NaOH/EtOH) at variable wavelength offsets (Δλ 15–210 nm) at 77K; Figure S7: (a) Absorbance of chalcone 2 (2.5 μM) in EtOH (black) and 5 mM NaOH in EtOH (blue). (b) Excitation (dotted lines) and fluorescence (solid lines) of chalcone 2 (2.5 μM) in EtOH (black) and 5 mM NaOH in EtOH (blue) at room temperature; Figure S8: Absorbance (dotted lines) and fluorescence emission (solid lines) spectra of chalcone 2 (2.5 μM) in 5 mM NaOH/EtOH before (0 equiv, black) and after incremental addition of HCl (1–4 equiv relative to NaOH); Figure S9. Synchronous fluorescence spectra of chalcone 2 (2.5 μM) at room temperature in EtOH (left) and 5 mM NaOH/EtOH (right) acquired at variable wavelength offsets, Δλ = 35–205 nm; Figure S10. Excitation (dotted) and emission (solid) spectra of 2 (2.5 μM) in 5 mM NaOH/EtOH at 77 K; Figure S11. Excitation (dotted) and emission (solid) spectra of 2 (2.5 μM) in 5 mM NaOH/EtOH after acidification with 4 equivalents of HCl at 77 K; Figure S12. Synchronous fluorescence spectra of chalcone 2 (2.5 μM) at 77 K in EtOH (left) and 5 mM NaOH/EtOH (right) acquired at variable wavelength offsets, Δλ = 26–205 nm; Table S1. Summary of the excitation and fluorescence peaks of 2 in wavelength (nm) and frequency (cm^{-1}).

Author Contributions Statement: Y.P. and B.C. proposed concept. B.C., M.H. and A. D. D. Z. participated the synthesis and low temperature fluorescence study. M.H. and B.C. prepared Figures 1-3. A. D. D. Z. prepared Figures 4–6. Y.P. and B.C. wrote the main manuscript text. All authors reviewed the manuscript.

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Competing interests: The authors declare no competing interests.

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