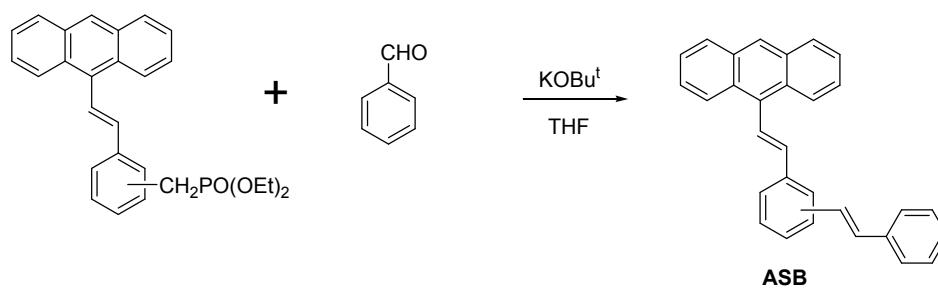


Supporting Information

Effect of Substitution Position on Crystal Packing, Polymorphism and Crystallization-Induced Emission of (9-Anthryl)vinylstyrylbenzene Isomers

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e S1 Synthetic routes to the three isomers.

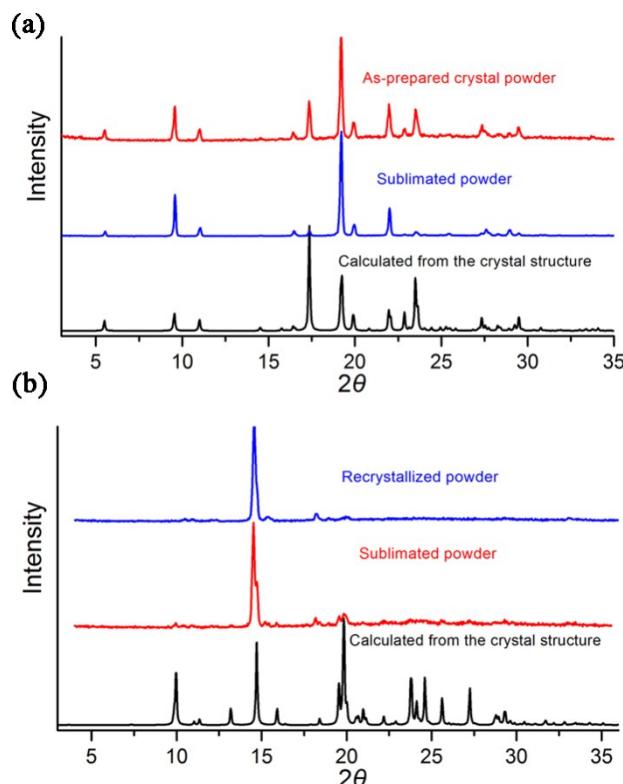


Fig. S1 XRD patterns of 1,2-ASB (a) and 1,4-ASB (b).

Table S1. Crystal data and details of collection and refinement for the three isomers.

Compound	1,2-ASB	1,3-ASB- β	1,4-ASB
Chemical formula	C ₃₀ H ₂₂	C ₃₀ H ₂₂	C ₃₀ H ₂₂
Formula Mass	382.48	382.48	382.48
Crystal system	Orthorhombic	Monoclinic	Triclinic
<i>a</i> /Å	32.3617(7)	22.1305(4)	9.3498(16)
<i>b</i> /Å	18.5058(5)	5.90728(9)	9.4481(18)
<i>c</i> /Å	7.04172(13)	33.8663(6)	24.396(2)
α /°	90.00	90.00	89.902(12)
β /°	90.00	106.7088(18)	81.207(12)
γ /°	90.00	90.00	76.231(16)
Unit cell volume/Å ³	4217.15(16))	4240.44(12)	2067.2(6)
Temperature/K	293.15	293.15	293.15
Space group	<i>Pccn</i>	<i>P2/c</i>	<i>P-1</i>
No. of formula units per unit cell, <i>Z</i>	8	8	4
$\rho_{\text{calcd}} / \text{g cm}^{-3}$	1.205	1.198	1.229
No. of reflections measured	15855	23097	9472
No. of independent reflections	3729	7454	5152
R_{int}	0.0218	0.0280	0.0460
Final R_I values ($I > 2\sigma(I)$)	0.0484	0.0448	0.1011
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1275	0.1093	0.2633
Final R_I values (all data)	0.0624	0.0677	0.1684
Final $wR(F^2)$ values (all data)	0.1403	0.1224	0.3295
Goodness of fit on F^2	1.027	1.023	1.027

Compound 1,4-ASB is inclined to grow into needle or thin-plate crystals, which is possibly related to the lamellar packing in the crystal structure. The diffraction intensity of these crystals, especially in the high diffraction angle, is weak. This brings difficulty to determine the crystal structure and the data are not satisfying in comparison with those of 1,2-ASB and 1,3-ASB- β .

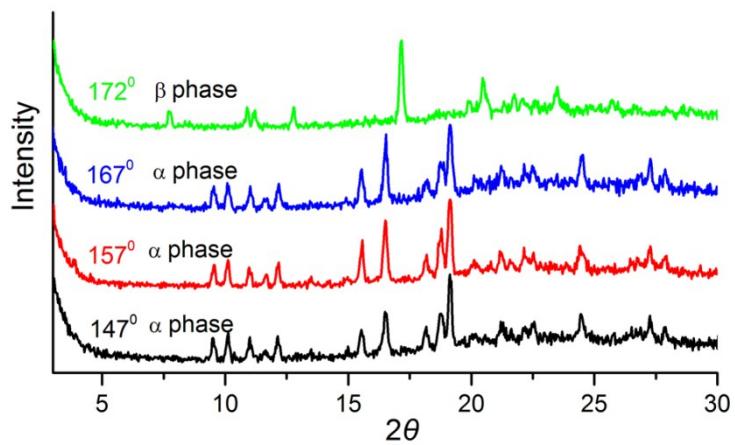


Fig. S2 The change of XRD patterns of 1,3-ASB as-prepared powder with temperature.

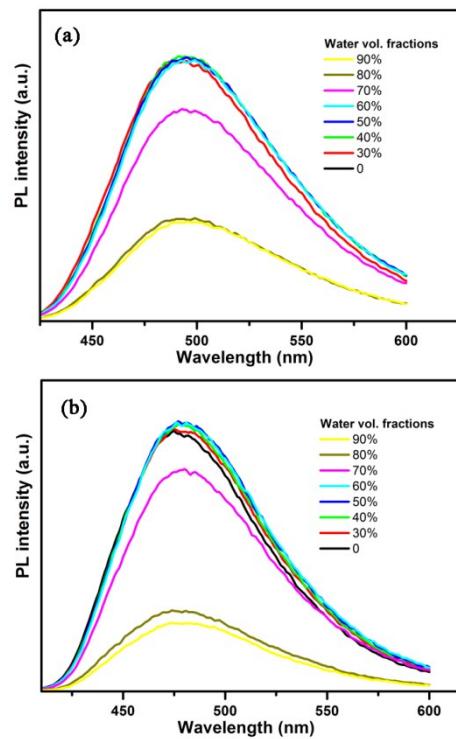


Fig. S3 PL spectra of 1,2-ASB (a) and 1,3-ASB (b) in THF/water mixtures with different water volume fractions. The concentration is 1×10^{-5} M.

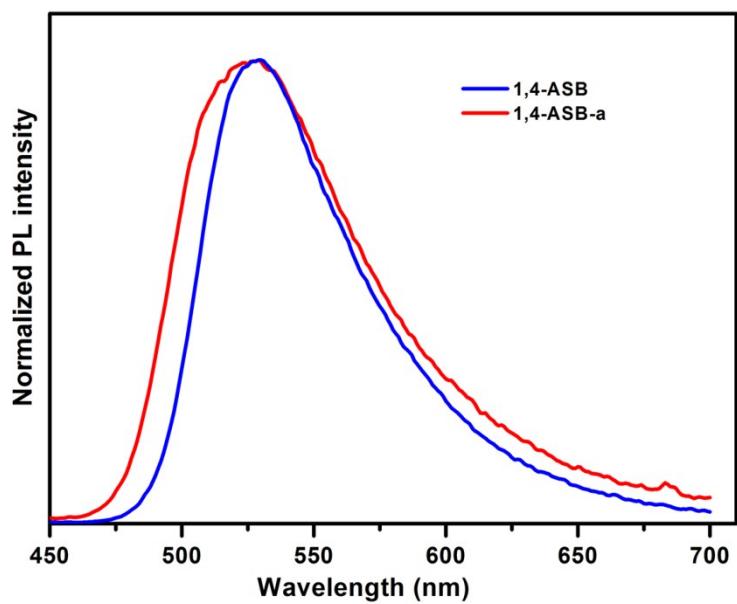


Fig. S4 The emission spectra of 1,4-ASB and 1,4-ASB-a samples.