Electronic Supplementary Material (ESI) for CrystEngComm.

<Electronic supplementary information (ESI)>

Adsorption of anthracene substitutes into suprachannels: bulk vs included guests

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Refinements of structures with the SQUEEZE routine in *PLATON*

For $[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$, one of the three counteranions and solvate molecules in the voids were highly disordered and were impossible to refine using conventional discrete-atom model. The terminal pyridyl groups combined with the amide moiety can rotate freely through the single bond, and thus, they seem to induce the statistical disorder of the structure. Therefore, the residual electron density was treated as diffuse contributions using the SQUEEZE of the PLATON software and located a series of voids.

For $[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$,

_platon_squeeze_void_nr

_platon_squeeze_void_average_x

_platon_squeeze_void_average_y

_platon_squeeze_void_average_z

_platon_squeeze_void_volume

_platon_squeeze_void_count_electrons

_platon_squeeze_void_content

1 -0.003 -0.003 -0.006 9497 2507 ' '

2 0.500 -0.002 0.250 121 30 ' '

3 0.500 0.002 0.750 116 30 ' '

4 0.000 0.498 0.250 121 30 ' '

5 0.000 0.502 0.750 116 30 ' '

_platon_squeeze_void_probe_radius 1.20

_platon_squeeze_details ?

Table S1. Fluorescence lifetime (nm) of 9,10-H_2ANT and 9,10-$(EtO)_2$ANT in 9,10-H_2ANT-⊂$[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$, 9,10-$(EtO)_2$ANT⊂$[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$, and 9,10-$H_2$ANT·9,10-$(EtO)_2$ANT⊂$[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$ in the solid-state at room temperature.

	λ_{em}	τ_1	τ_2	τ_3	τ_m
9,10-H_2ANT ⊂$[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$	409 nm	0.81	3.7	12	7.81
9,10-$(EtO)_2$ANT ⊂$[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$	450 nm	2.3	12.2	78	13
9,10-H_2ANT·9,10-$(EtO)_2$ANT ⊂$[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$	406 nm	0.66	2.66	7.8	3.31
	450 nm	2.9	14	90	16

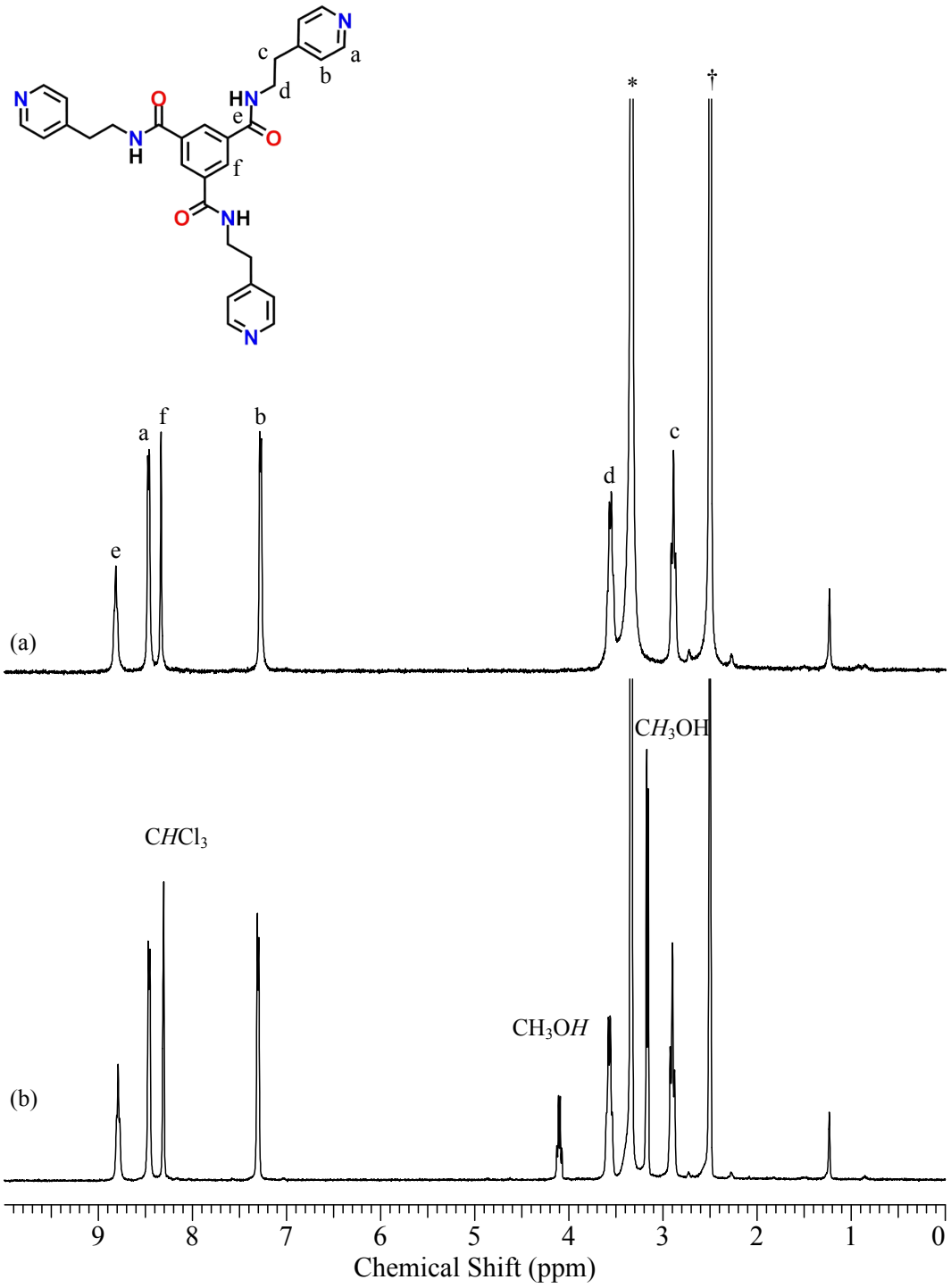


Fig. S1. ^{1}H NMR spectra (in Me_2SO-d_6) of L (a) and $[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$ (b), indicating that the complex is fully dissociated in Me_2SO.

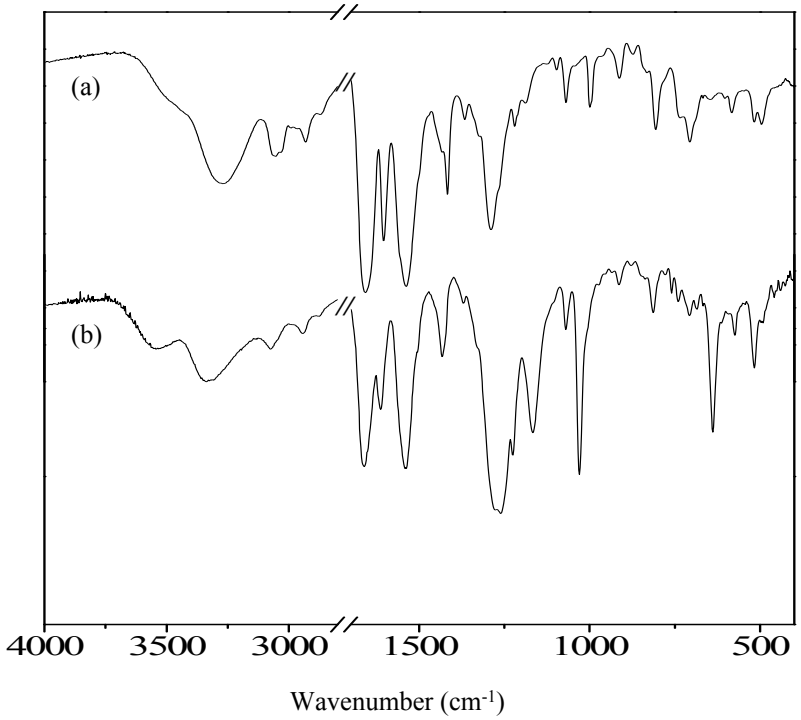


Fig. S2. FT-IR spectra of L (a) and $[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$ (b).

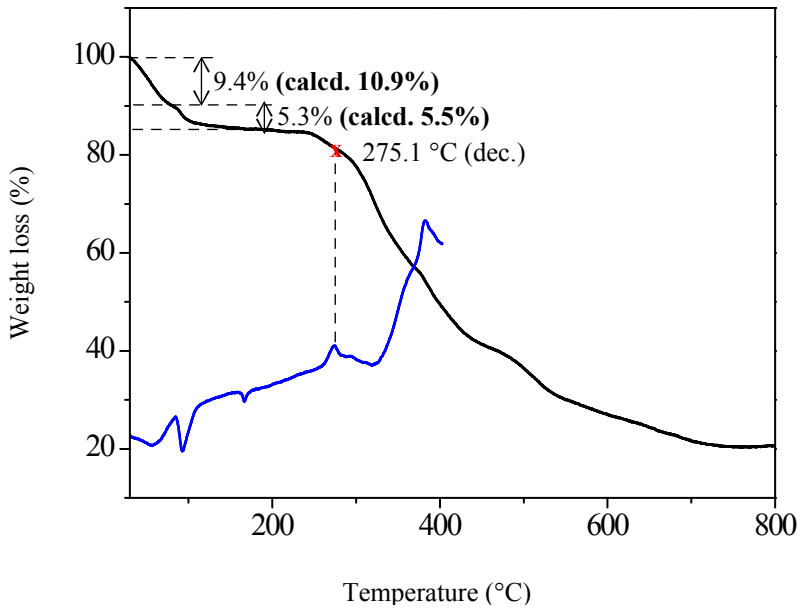
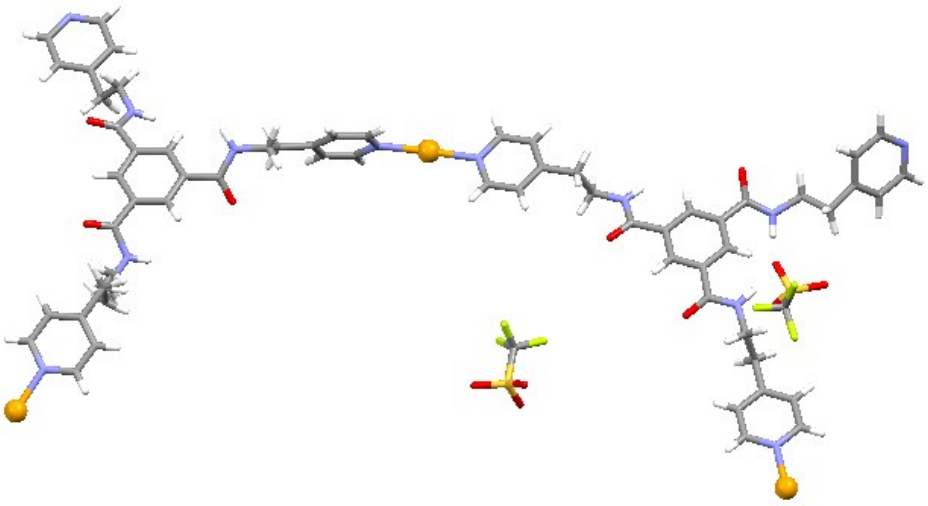


Fig. S3. TGA (black line) and DSC (blue) curves of $[Ag_3L_2]$ $(OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$. Weight loss: calcd, 10.9%; found, 9.4% ($2CHCl_3$); calcd, 5.5%; found, 5.3% ($4CH_3OH$); dec. temp. of skeleton: 271.5 °C.

(a)



(b)

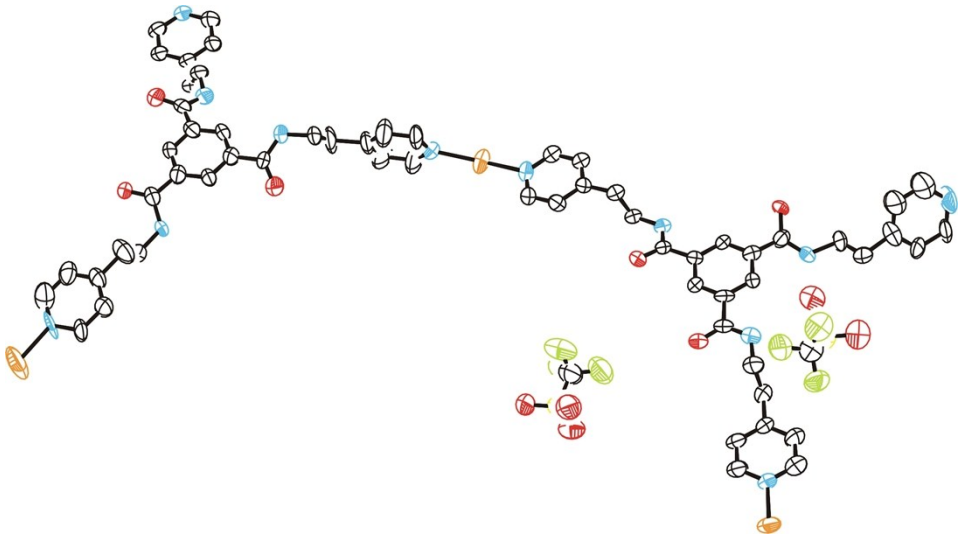


Fig. S4. Coordination views: Ball-and-stick (a) and ORTEP (b).

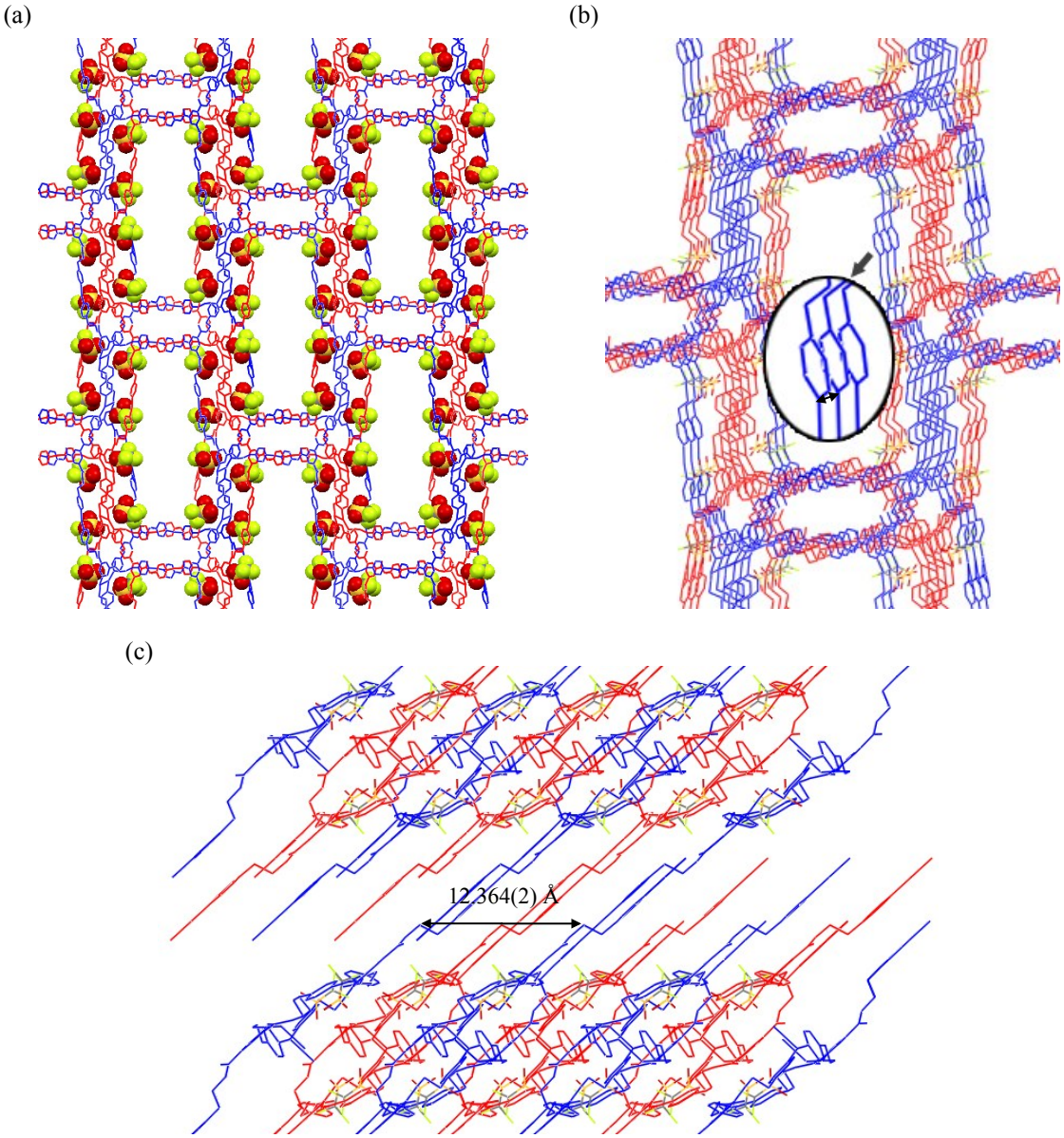


Fig. S5. Crystal structure of $[Ag_3L_2](OTf)_3 \cdot 4CH_3OH \cdot 2CHCl_3$: (a) packing structure of 2D channels, (b) top views and (c) side views.

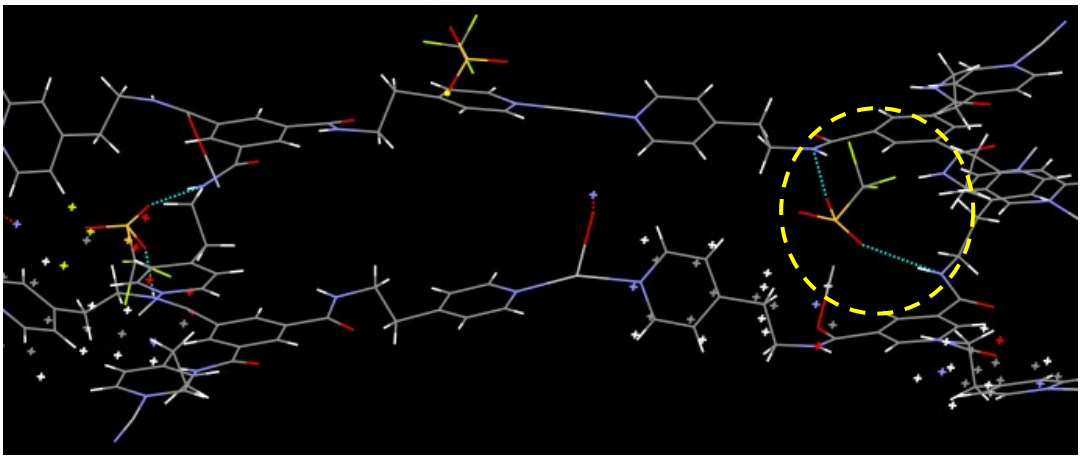


Fig. S6. Crystal structure of the triflate anions bridge between two amide groups.

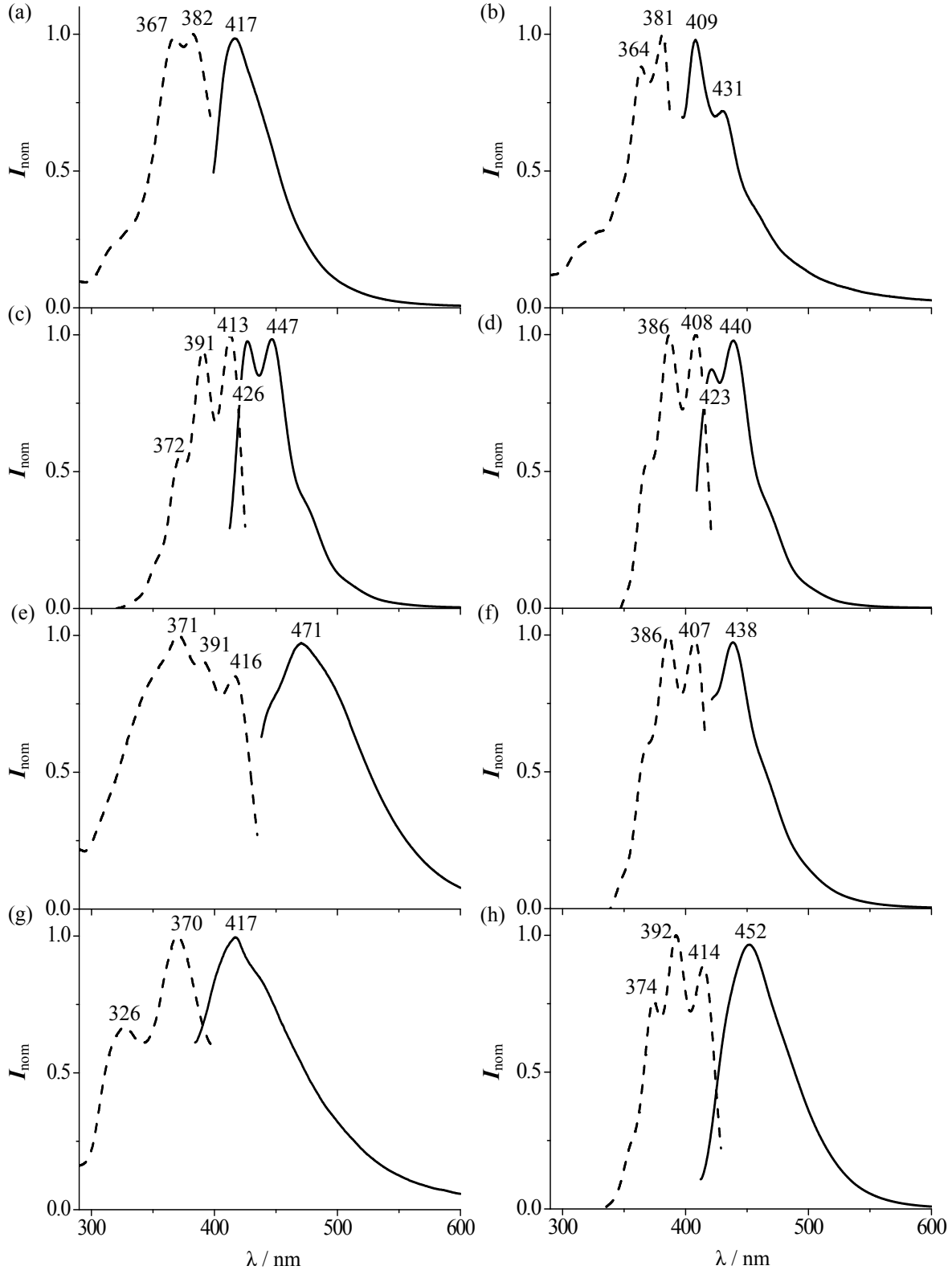


Fig. S7. Solid-state excitation spectra (dashed line) and emission spectra (solid line) of $AS\subset[Ag_3L_2](OTf)_3\cdot 4CH_3OH\cdot 2CHCl_3$. a) ANT; b) 9,10-$H_2$ANT; c) 9,10-$Br_2$ANT; d) 9,10-$Cl_2$ANT; e) 9,10-$(ClMe)_2$ANT; f) 9,10-$Me_2$ANT; g) 9,10-$(NC)_2$ANT; h) 9,10-$(EtO)_2$ANT.