

Steric Control over Supramolecular Polymer Formation in *trans*-1,2-Bis(4-pyridyl)ethylene Adducts of Zinc Xanthates: Implications for Luminescence

Jun-Gill Kang, Dong-Hee Cho, Yong-Kwang Jeong, Changmoon Park, Shu Fang Soh, Chian Sing Lai, and Edward R. T. Tiekink

*** SUPPORTING MATERIALS ***

Figure S1. Polymeric strands in $\{\text{Zn}(\text{S}_2\text{COEt})_2\text{L}\}_\infty$ (**1**) and $\{\text{Zn}(\text{S}_2\text{COBu})_2\text{L}\}_\infty$ (**2**) represented in space filling mode.

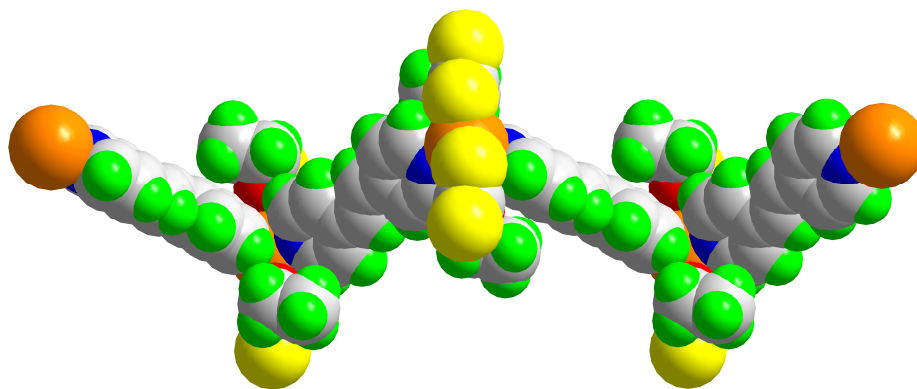
Figure S2. Views of the layers and global crystal packing in $\{\text{Zn}(\text{S}_2\text{COEt})_2\text{L}\}_\infty$ (**1**) and $\{\text{Zn}(\text{S}_2\text{COBu})_2\text{L}\}_\infty$ (**2**).

Figure S3. Crystal packing in $\{[\text{Zn}(\text{S}_2\text{COCy})_2]_2\text{L}\}$ (**3**).

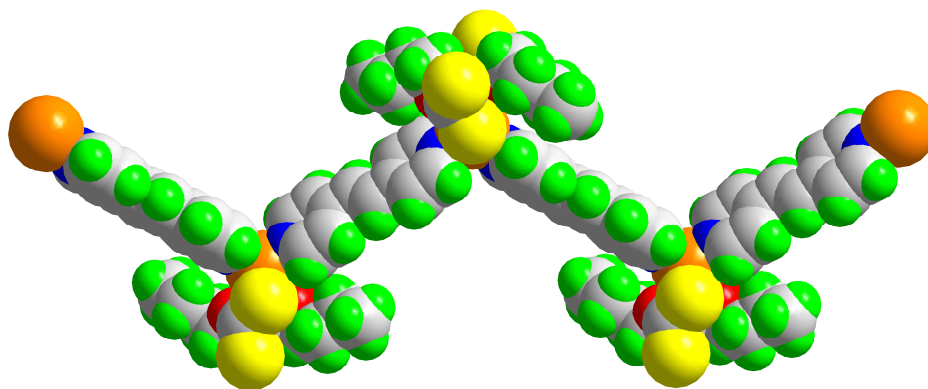
Table S1. Experimental and calculated bond lengths (Å) and angles (°) for $\{[\text{Zn}(\text{S}_2\text{COCy})_2]_2\text{L}\}$

Table S2. CI excited states with high oscillator strength and predominant transitions for $\{[\text{Zn}(\text{S}_2\text{COCy})_2]_2\text{L}\}$

Table S3. CI excited states with high oscillator strength and predominant transitions for $\text{Zn}(\text{S}_2\text{COCy})_2$

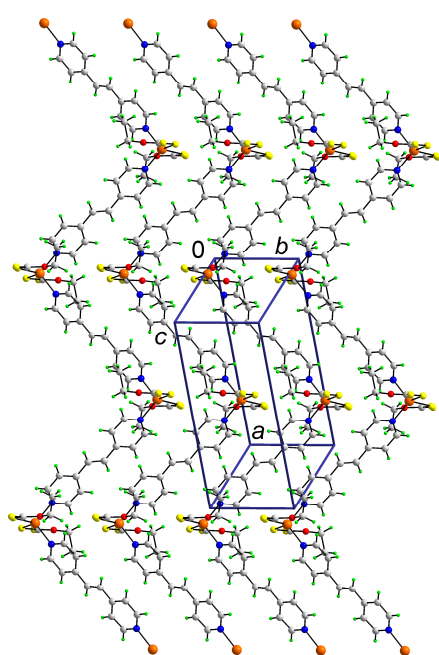


(1)

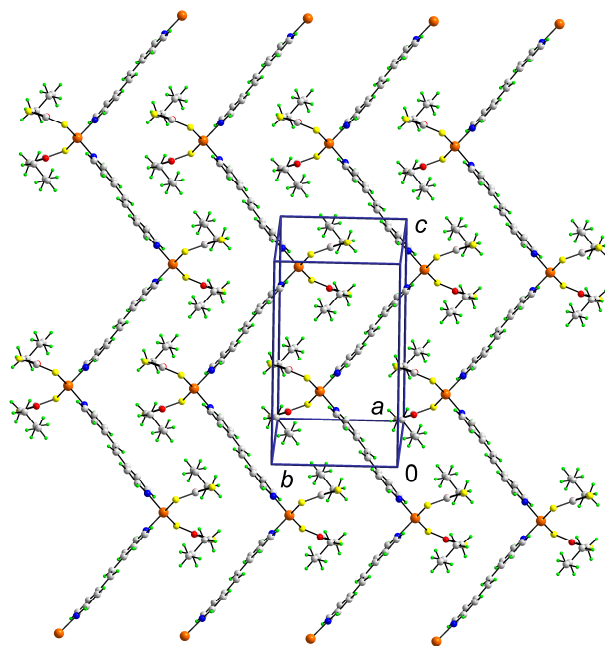


(2)

Figure S1. Polymeric strands in $\{\text{Zn}(\text{S}_2\text{COEt})_2\text{L}\}_\infty$ (1) and $\{\text{Zn}(\text{S}_2\text{COBu})_2\text{L}\}_\infty$ (2) represented in space filling mode.



(1)



(2)

Figure S2. Views of the layers and global crystal packing in $\{\text{Zn}(\text{S}_2\text{COEt})_2\text{L}\}_\infty$ (1) and $\{\text{Zn}(\text{S}_2\text{COBu})_2\text{L}\}_\infty$ (2).

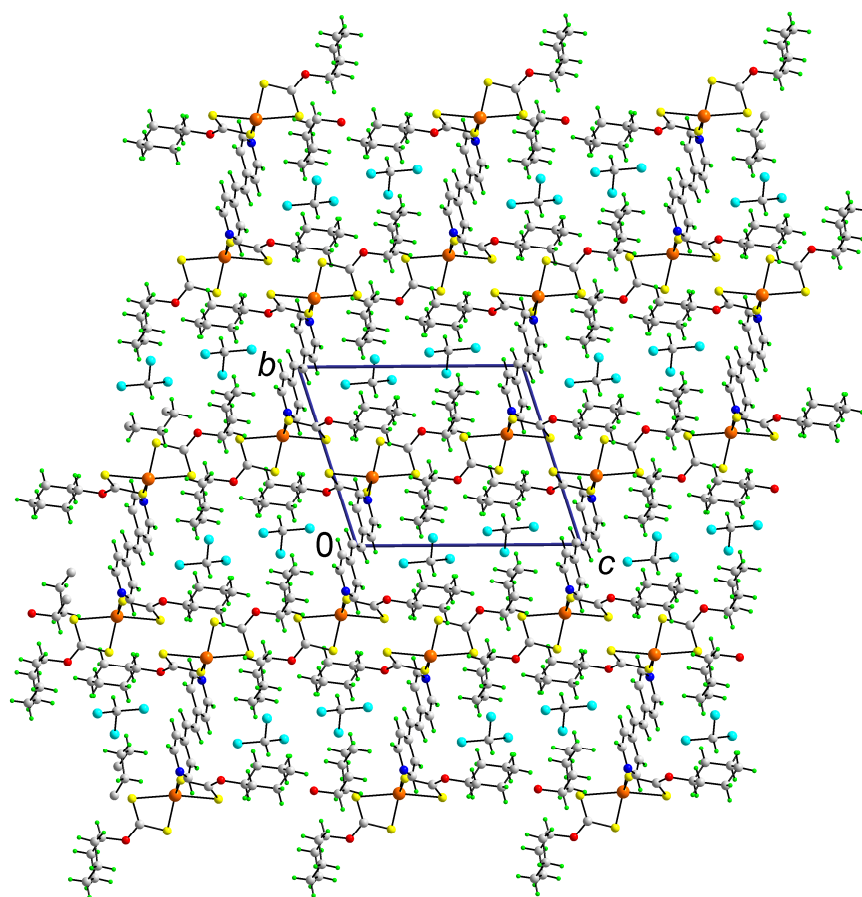


Figure S3. Crystal packing in $\{[\text{Zn}(\text{S}_2\text{COCy})_2]_2\text{L}\}$ (**3**).

**Table S1. Experimental and calculated bond lengths (Å) and angles (°) for
{[Zn(S₂COCy)₂]₂L}**

	Expt.*	Calc.		Expt.*	Calc.
Zn-S1, Zn-S3	2.325	2.408	Zn-S2, Zn-S4	2.624	2.7211
Zn-N1	2.044	2.100	S1-Zn-S2, S3-Zn-S4	73.2	70.9
S1-Zn-S4, S2-Zn-S3	101.0	105.2	S1-Zn-N1, S3-Zn-N1	112.7	105.0
S2-Zn-S4	165.3	169.3	S2-Zn-N1, S4-Zn-N1	97.3	95.3

*Average of two values.

Table S2. CI excited states with high oscillator strength and predominant transitions for {[Zn(S₂COCy)₂]₂L}

Excited state	eV	Oscillator strength, <i>f</i>	Main transition
1B	5.69	0.012	$h2 \rightarrow l3, h1 \rightarrow l2$
1A	5.68	0	$h2 \rightarrow l2, h1 \rightarrow l3$
2A	5.73	0	$h8 \rightarrow l2, h2 \rightarrow l5$
2B	5.73	0	$h8 \rightarrow l3, h1 \rightarrow l5$
3B	6.21	0.463	$h4 \rightarrow l3, h3 \rightarrow l2$
3A	6.21	0	$h4 \rightarrow l2, h3 \rightarrow l3$
4B	6.26	1.670	$h9 \rightarrow l1$
4A	6.35	0.027	$h6 \rightarrow l2$
5B	6.35	0.318	$h6 \rightarrow l3, h5 \rightarrow l2$
5A	6.54	0	$h4 \rightarrow l10, h3 \rightarrow l11$
6B	6.54	0.002	$h4 \rightarrow l11, h3 \rightarrow l10$
6A	6.58	0	$h6 \rightarrow l10, h5 \rightarrow l11$
7B	6.58	0.080	$h6 \rightarrow l11, h5 \rightarrow l10$
7A	6.66	0	$h2 \rightarrow l10, h1 \rightarrow l11$
8B	6.67	0.007	$h2 \rightarrow l11, h1 \rightarrow l10$
9B	6.79	0.030	$h1 \rightarrow l17, h7 \rightarrow l10$
8A	6.79	0.016	$h8 \rightarrow l10, h2 \rightarrow l17$
9A	6.93	0	$h21 \rightarrow l2, h20 \rightarrow l3$
10B	6.93	0	$h22 \rightarrow l3, h21 \rightarrow l2$
10A	6.94	0.004	$h22 \rightarrow l5, h21 \rightarrow l4$
11B	6.94	0.005	$h21 \rightarrow l5$
11A	7.01	0	$h15 \rightarrow l1$
12B	7.02	0.233	$h14 \rightarrow l1$
13B	7.41	0	$h10 \rightarrow l13, h11 \rightarrow l2$
12A	7.42	1.140	$h10 \rightarrow l2, h11 \rightarrow l3$
14B	7.46	0.060	$h13 \rightarrow l3, h12 \rightarrow l2$

Table S3. CI excited states with high oscillator strength and predominant transitions for $\text{Zn}(\text{S}_2\text{COCy})_2$

Excited state	eV	Oscillator strength, f	Main transition
1B	5.92	0	$h3 \rightarrow l2, h2 \rightarrow l1$
1A	5.94	0	$h3 \rightarrow l1, h2 \rightarrow l2$
2B	6.23	0.062	$h1 \rightarrow l2, h1 \rightarrow l3$
2A	6.24	0.075	$h1 \rightarrow l1$
3B	6.33	0.022	$h1 \rightarrow l3$
3A	6.34	0.001	$h4 \rightarrow l3$
4B	6.64	0.063	$h3 \rightarrow l3$
4A	6.65	0.053	$h2 \rightarrow l3, h4 \rightarrow l3$
5B	6.88	0.005	$h13 \rightarrow l2, h8 \rightarrow l1$
5A	6.90	0	$h13 \rightarrow l1, h8 \rightarrow l2$
6B	7.43	0.676	$h6 \rightarrow l1, h5 \rightarrow l2$
6A	7.45	0.015	$h5 \rightarrow l1, h6 \rightarrow l2$
7B	7.51	0.114	$h5 \rightarrow l3, h1 \rightarrow l2$
7A	7.52	0.005	$h5 \rightarrow l7$
8B	7.72	0.098	$h5 \rightarrow l3, h4 \rightarrow l7$
8A	7.74	0.091	$h6 \rightarrow l3, h4 \rightarrow l2$
9A	7.87	0	$h1, h7 \rightarrow l1$
9B	7.91	0.033	$h7 \rightarrow l2$