# Electronic Supplementary Information

# Stereochemically active and inactive lone pairs in two room temperature phosphorescence coordination polymers of $Pb^{2+}$ with different tricarboxylic acids

Xu-Sheng Gao,*[a] Hai-Jie Dai,[a] Mei-Juan Ding,[a] Wen-Bo Pei,[a] Xiao-Ming Ren*[a,b]

[a] State Key Laboratory of Materials–Oriented Chemical Engineering and College of Chemistry & Molecular Engineering, Nanjing Tech University, Nanjing 211816, P. R. China

[b] State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, P. R. China

Tel: +86 25 58139527
Fax: +86 25 58139988
Email: gaoxs@njtech.edu.cn (XSG)
xmren@njtech.edu.cn (XMR)

**Contents**

Table S1: Selected bond length (Å) and bond angle ( ) for **1** and **2**

| | | | |
|---|---|---|---|
| **1** | | | |
| Bond length / Å | | | |
| Pb1#3-O5 | 2.421(4) | Pb1-O2 | 2.560(3) |
| Pb1#3-O6 | 2.610(4) | Pb1#2-O2 | 2.623(3) |
| Pb1#1-O1 | 2.584(4) | Pb1-O7 | 2.749(12) |
| Bond angles / ° | | | |
| O5#4-Pb1-O2 | 83.69(12) | O5#4-Pb1-O1#2 | 73.97(13) |
| O5#4-Pb1-O6#4 | 51.98(12) | O2-Pb1-O6#4 | 133.79(12) |
| O5#4-Pb1-O2#1 | 90.38(13) | O2-Pb1-O2#1 | 114.45(8) |
| O6#4-Pb1-O2#1 | 81.93(11) | O5#4-Pb1-O7 | 150.1(3) |
| O1#2-Pb1-O7 | 78.6(3) | O6#4-Pb1-O7 | 135.8(3) |
| Pb1-O2-Pb1#2 | 108.84(12) | O1#2-Pb1-O6#4 | 82.96(11) |
| O2-Pb1-O1#2 | 71.39(10) | O2#1-Pb1-O7 | 118.1(3) |
| O2-Pb1-O7 | 76.4(3) | O1#2-Pb1-O2#1 | 162.91(12) |
| Symmetry codes: #1 = 1/2-*x*, -1/2+*y*, 1/2-*z*; #2 =1/2-*x*, 1/2+*y*, 1/2-*z*; #3 =+*x*, 2-*y*, -1/2+*z*; #4 =1-*x*, +*y*, 1/2-*z* | | | |
| **2** | | | |
| Bond length / Å | | | |
| Pb1-O1 | 2.427(5) | Pb1-O2#2 | 2.618(6) |
| Pb1-O5#1 | 2.610(5) | Pb1-O6 | 2.567(6) |
| Pb1-N1 | 2.452(7) | | |
| Bond angles / ° | | | |
| O1-Pb1-N1 | 66.2(2) | N1-Pb1-O5#1 | 78.5(2) |
| O1-Pb1-O5#1 | 78.29(19) | N1-Pb1-O2#2 | 76.2(2) |
| O1-Pb1-O2#2 | 103.82(18) | N1-Pb1-O6 | 64.70(19) |
| O5#1-Pb1-O2#2 | 150.91(19) | O6-Pb1-O5#1 | 84.16(18) |
| O1-Pb1-O6 | 130.10(18) | O6-Pb1-O2#2 | 72.28(18) |
| Symmetry codes: #1 = 1/2–*x*, -1/2+*y*, 1/2-*z*; #2 = +*x* ,1+*y*, +*z* | | | |

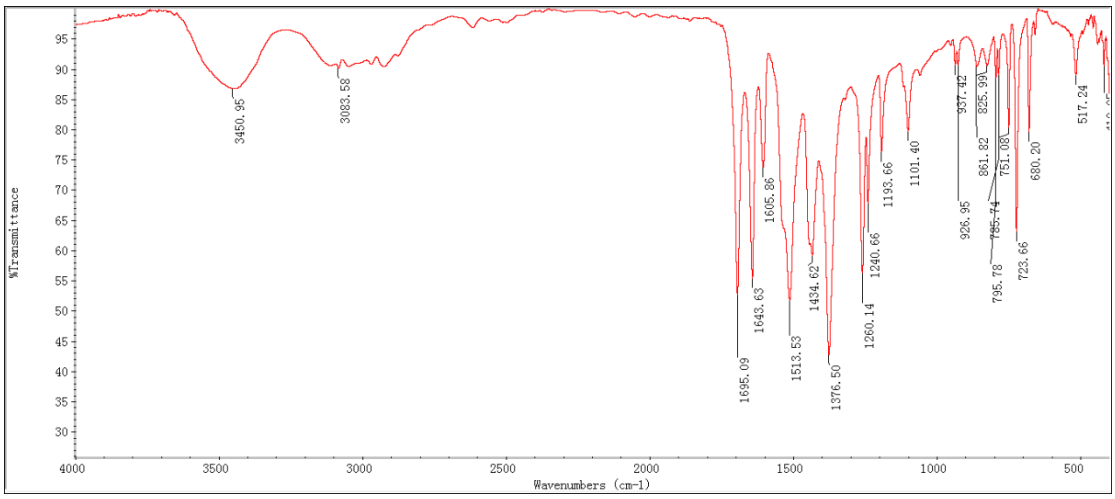


**Fig. S1** IR spectrum of **1**

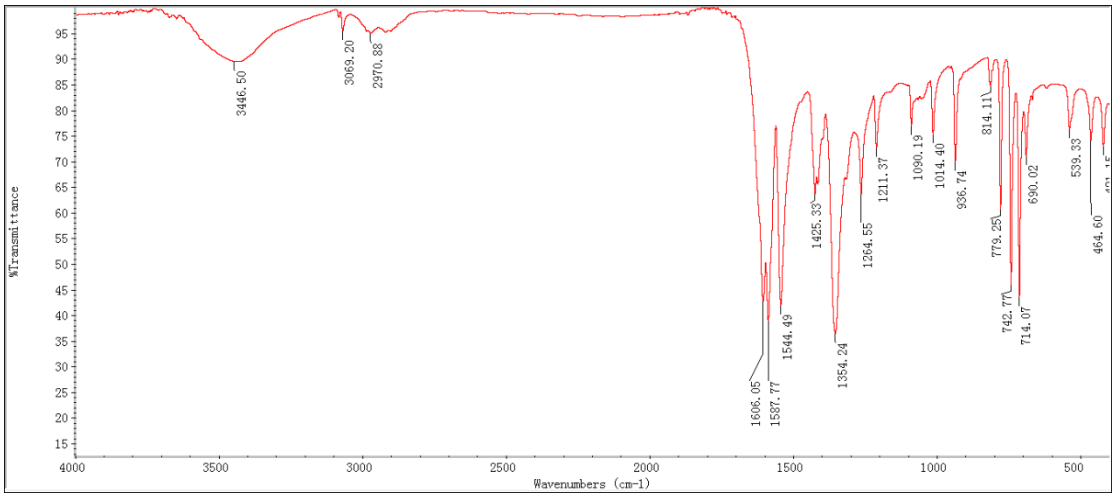


**Fig. S2** IR spectrum of **2**

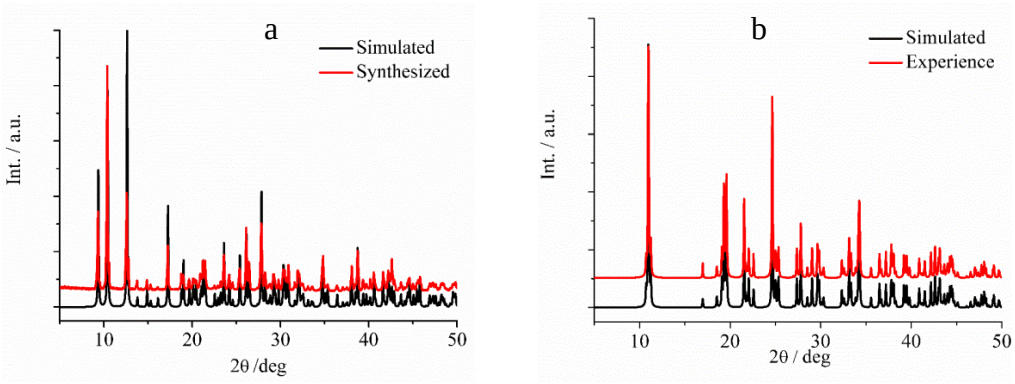


**Fig. S3** (a) The powder X-ray diffraction patterns for **1**. (b) Powder X-ray diffraction patterns of **2**.

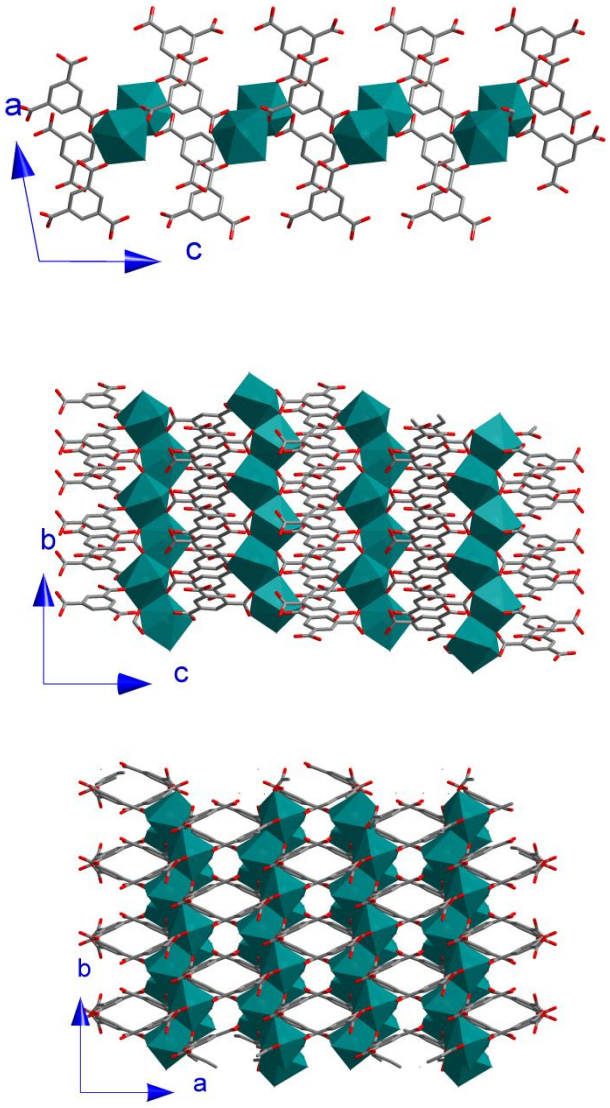


**Fig. S4** Packing diagram of **1** viewed along *c*-axis.

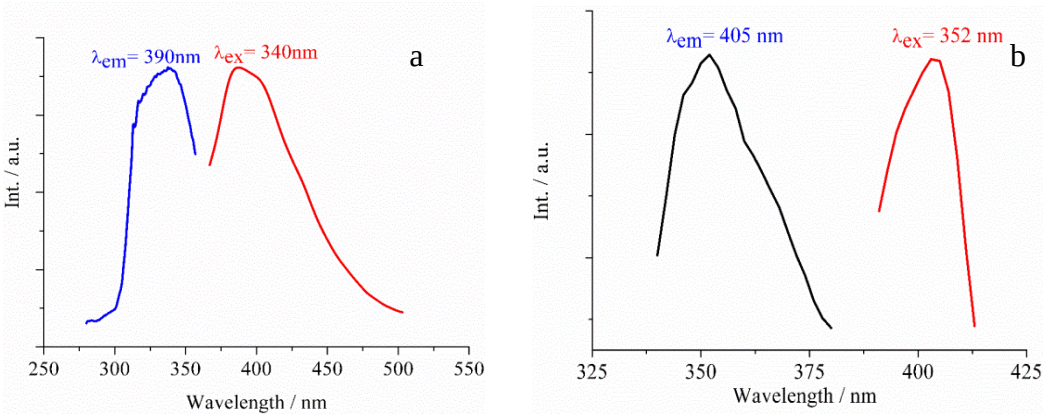


**Fig. S5** (a) Excited and emission spectra of $H_3BTC$ at ambient temperature. (b) Excited and emission spectra of $H_3PTC$ at ambient temperature.

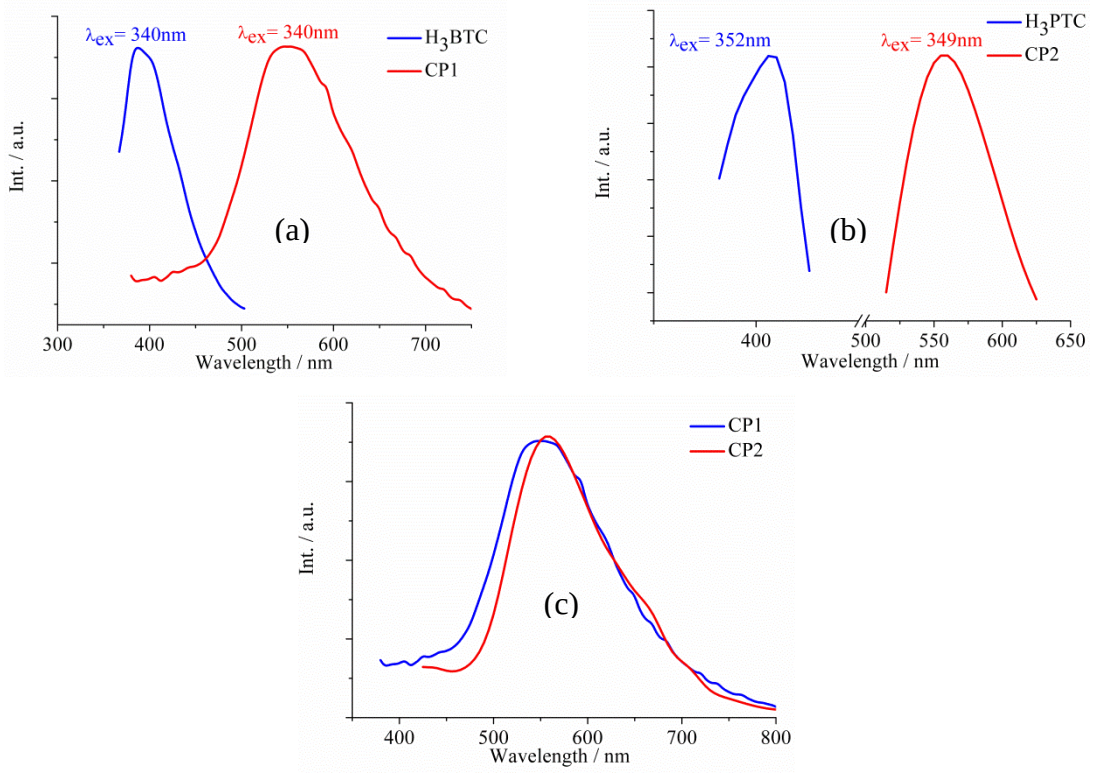


**Fig. S6** (a) Emission spectra of $H_3BTC$ and **1** at ambient temperature. (b) Emission spectra of $H_3PTC$ and **2** at ambient temperature. (c) Emission spectra of **1** and **2** at ambient temperature.

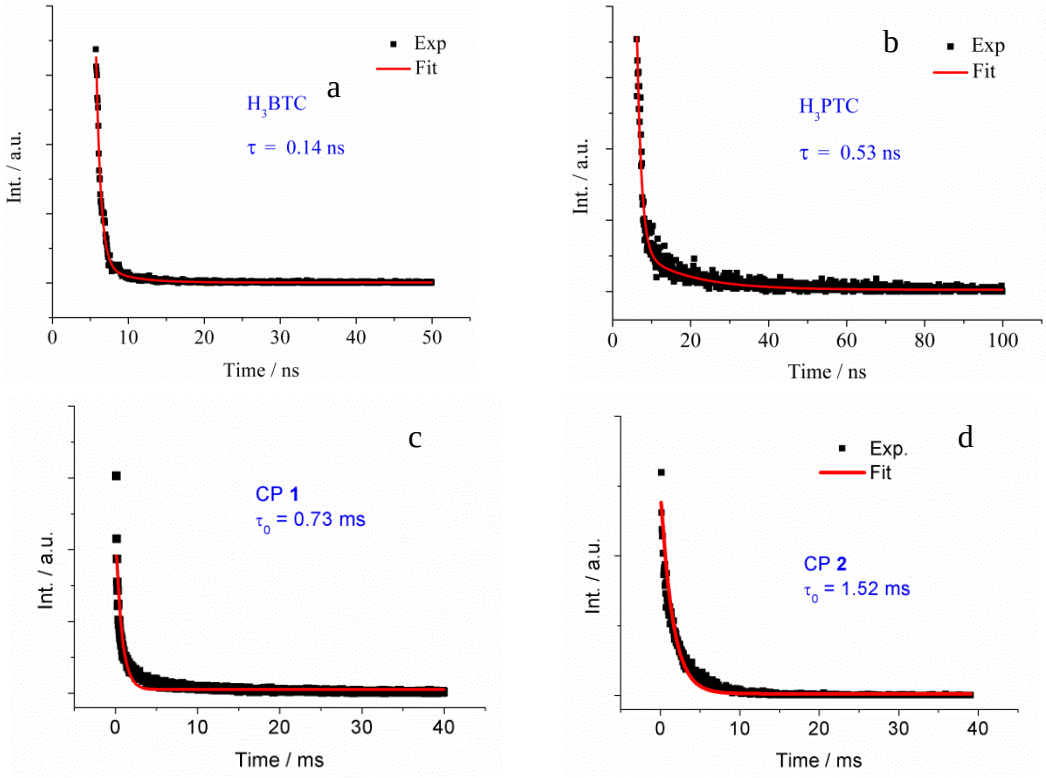


**Fig. S7** Emission decay of (a) $H_3$BTC and (b) $H_3$PTC obtained at room temperature upon pulsed excitation at 340 nm and 352 nm, where the red lines and the black squares represent the fitting curves and the experimental data, respectively. Emission decay of (c) **1** and (d) **2** obtained at room temperature upon pulsed excitation at 355 nm, where the red lines and the black squares represent the fitting curves and the experimental data, respectively.