Photoluminescence and self-assembly of three different Eu complexes

Supplementary information

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1 Availability of raw data.

The raw data of STM topography images and photoluminescence measurements has been uploaded to Zenodo, DOI: 10.5281/zenodo.15920446.

2 Synthetic Procedures

Materials: 2-Thenoyltrifluoroacetone (TTFA, 99%) and 2,2'-bipyridine were purchased from Sigma Aldrich. EuCl3·6 H_2O (99,9%) a) were purchased from abcr. IR spectra were recorded on a Bruker Tensor 37 FTIR spectrometer equipped with a DLaTGS detector, a diamond ATR (attenuated total reflection) unit and a nitrogen flushed chamber.

3 Synthesis of $[Eu(tta)_3(H_2O)_2]$ [1]

1.33 g of 2-thenoyltrifluoroacetone (5.99 mmol, 3.00 eq.) was dissolved in 30 mL absolute ethanol. Then, 6 mL of 1 N NaOH and 0.73 g of $EuCl_3 \cdot 6H_2O$ (1.99 mmol, 1.00 eq.), dissolved in 10 mL deionized H_2O, were added. After heating to 60 °C, 200 mL deionized H_2O was slowly added. The precipitated complex was vacuum filtered, washed with deionized H_2O, and vacuum dried to yield a yellow powder. Details of the synthesis and the analytical data, was published recently by us[2].

4 Synthesis of $[Eu(tta)_3(bpy)]$ [3]

665 mg of 2-thenoyltrifluoroacetone (2.99 mmol, 3.00 eq.) and 156 mg of 2,2'-bipyridine (0.99 mmol, 1.00 eq.) were dissolved in 15 mL of absolute ethanol. After adding 2 mL of 1 N KOH, the solution was heated to 60 °C. Separately, 365 mg of $EuCl_3 \cdot 6H_2O$ (0.99 mmol, 1.00 eq.) was dissolved in 5 mL of deionized H_2O and added dropwise to the heated solution. The resulting precipitate was collected via vacuum filtration, washed with deionized H_2O, and dried under vacuum, yielding a light-yellow powder. Lattice constants of single crystals (a = 10.3145(8), b = 16.3996(14), c = 21.8106(16), $\alpha = 90$, $\beta = 103.068(6)$, $\gamma = 90$, V = 3593.8(5), space group $P2_1/n$) match with the literature[4].

5 Synthesis of $[Eu(btfa)_3(bpy)]$ [5]

6 mmol of beta-diketone and 2,2'-bipyridine were dissolved in 20 ml ethanol and stirred at room temperature. A solution of NaOH was prepared by dissolving 0.24 mg of powdered NaOh in 2 ml H_2O The ethanolic solution containing [btfa] and NaOh was sirred and room temperature for over 2 h. 2mmol of $EuCl_36H_2O$ dissolved in 5 ml ethanol was added in the solution and the mixture was stirred at room temperature for additional 3 h. The experimentally found composition of $C_{40}H_{26}EuN_2F_9O_6$ closely matches the expected values: Calculated: C 50.58; H 2.75; N 2.94. Found: C 49.86; H 2.70; N 2.93.

References

[1] J. Kai, D. F. Parra and H. F. Brito, *Journal of Material Chemistry*, 2008, **18**, 4549–4554.

[2] J. Feye, J. Matthias, A. Fischer, D. Rudolph, J. Treptow, R. Popescu, J. Franke, A. L. Exarhos, Z. A. Boekelheide, D. Gerthsen, C. Feldmann, P. W. Roesky and E. S. Rösch, *Small*, 2023, **19**, 2301997.

[3] D. Chitnis, N. T. Kalyani and S. Dhoble, *Optik*, 2017, **130**, 237–244.

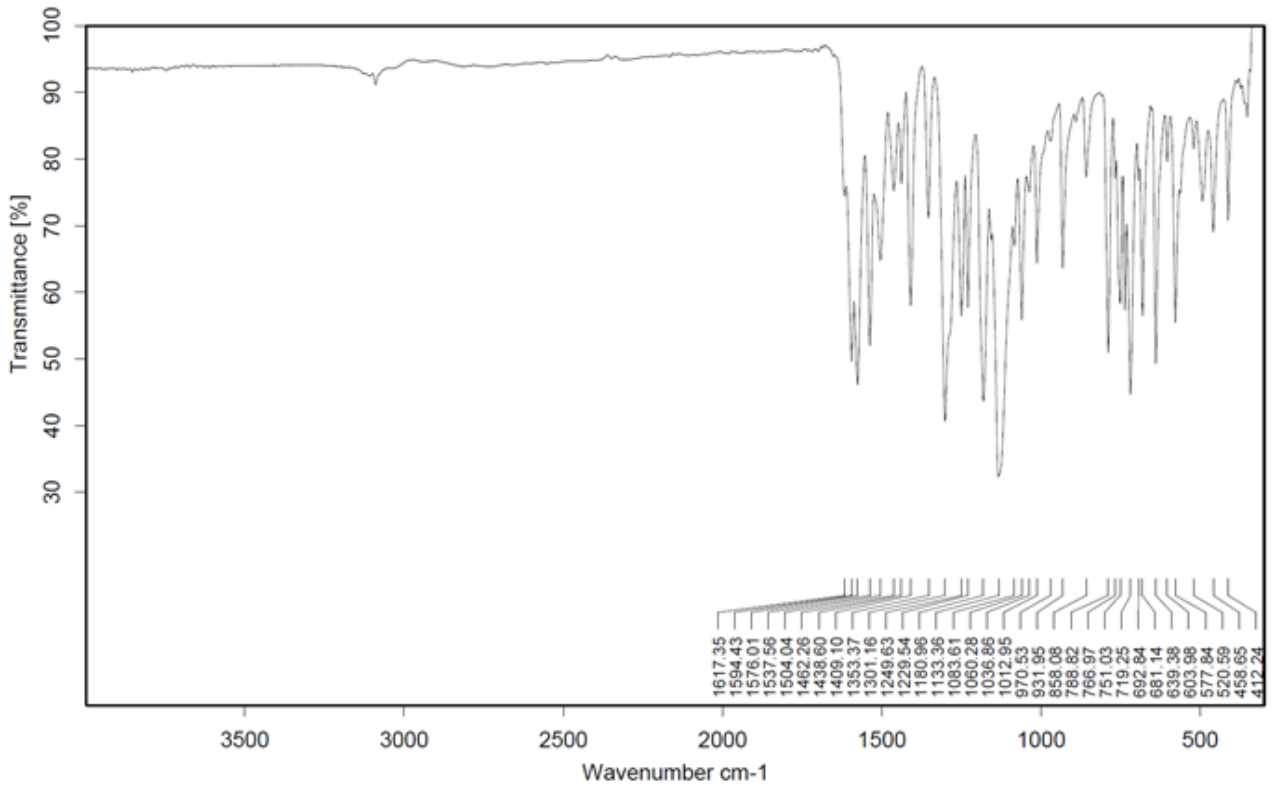

Figure 1: ATR IR spectra of $[Eu(tta)_3(bpy)]$.

[4] X.-F. Chen, X.-H. Zhu, Y.-H. Xu, S. Shanmuga Sundara Raj, S. Öztürk, H.-K. Fun, J. Ma and X.-Z. You, *Journal of Material Chemistry*, 1999, **9**, 2919–2922.

[5] H. J. Batista, A. V. M. de Andrade, R. L. Longo, A. M. Simas, G. F. de Sá, N. K. Ito and L. C. Thompson, *Inorganic Chemistry*, 1998, **37**, 3542–3547.