**Supporting Information**

**Triboluminescence of centrosymmetric lanthanide β-diketonate complexes with aggregation-induced emission**

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**Characterization and crystallography**



Figure S1. 1H NMR (400 Hz, CDCl3) spectra of *pp*-dbm-Cl2.



Figure S2. 13C NMR (100 Hz, CDCl3) spectra of *pp*-dbm-Cl2.



Figure S3. 1H NMR (400 Hz, CDCl3) spectra of *mm*-dbm-Cl2.



Figure S4. 13C NMR (100 Hz, CDCl3) spectra of *mm*-dbm-Cl2.



Figure S5. 1H NMR (400 Hz, CDCl3) spectra of [Eu(*pp*-dbm-Cl2)3phen].



Figure S6. 1H NMR (400 Hz, CDCl3) spectra of [Eu(*mm*-dbm-Cl2)3phen].

Table S1. Summary of crystal data and structure refinement.

|  |  |  |
| --- | --- | --- |
| Compound | [Eu(*pp*-dbm-Cl2)3phen] | [Eu(*mm*-dbm-Cl2)3phen] |
| Empirical formula | C57H35Cl6EuN2O6 | C57H35Cl6EuN2O6 |
| Formula weight | 1208.53 | 1208.53 |
| Temperature/K | 296(2) | 233(2) |
| Crystal system | monoclinic | monoclinic |
| Space group | *P*21/*n* | *P*21/*n* |
| a/Å | 14.2025(42) | 13.8631(6) |
| b/Å | 18.3534(52) | 16.6671(9) |
| c/Å | 20.3471(58) | 22.7611(11) |
| α/° | 90.00 | 90 |
| β/° | 93.6564(82) | 105.529(2) |
| γ/° | 90.00 | 90 |
| Volume/Å3 | 5293(3) | 5067.1(4) |
| Z | 4 | 4 |
| ρcalcg/cm3 | 1.517 | 1.584 |
| μ/mm‑1 | 1.540 | 1.609 |
| F(000) | 2416.0 | 2416.0 |
| Crystal size/mm3 | 0.28 × 0.28 × 0.20 | 0.54 × 0.31 × 0.12 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 4.88 to 55.74 | 4.446 to 52.78 |
| Index ranges | -18 ≤ h ≤ 18, -23 ≤ k ≤ 23, -25 ≤ l ≤ 26 | -16 ≤ h ≤ 17, -20 ≤ k ≤ 18, -28 ≤ l ≤ 25 |
| Reflections collected | 117171 | 42523 |
| Independent reflections | 12234 | 10366 |
| Data/restraints/parameters | 12234/0/650 | 10366/0/649 |
| Goodness-of-fit on F2 | 1.029 | 1.027 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0258, wR2 = 0.0568 | R1 = 0.0270, wR2 = 0.0570 |
| Final R indexes [all data] | R1 = 0.0369, wR2 = 0.0628 | R1 = 0.0377, wR2 = 0.0618 |
| Largest diff. peak/hole / e Å-3 | 0.59/-0.45 | 0.42/-0.56 |

**Photophysical measurement**



Figure S7. Excitation spectrum of [Eu(*pp*-dbm-Cl2)3phen] in THF



Figure S8. Excitation spectrum of [Eu(*mm*-dbm-Cl2)3phen] in THF



Figure S9. Luminescence decay curve at 5D0 → 7F2 transition of [Eu(*pp*-dbm-Cl2)3phen] in THF, 10 μM. Red line: biexponential fit curve.



Figure S10. Luminescence decay curve at 5D0 → 7F2 transition of [Eu(*mm*-dbm-Cl2)3phen] in THF, 10 μM. Red line: biexponential fit curve.



Figure S11. Emission spectrum of [Gd(*pp*-dbm-Cl2)3phen] in 2-methyltetrahydrofuran at 77 K.



Figure S12 Emission spectrum of [Gd(*mm*-dbm-Cl2)3phen] in 2-methyltetrahydrofuran at 77 K.



Figure S13. Luminescence decay curve at 5D0 → 7F2 transition of [Eu(*pp*-dbm-Cl2)3phen] solid. Red line: monoexponential fit curve.



Figure S14. Luminescence decay curve at 5D0 → 7F2 transition of [Eu(*mm*-dbm-Cl2)3phen] solid. Red line: monoexponential fit curve.



Figure S15. Image of [Eu(pp-dbm-Cl2)3phen] in THF/water with different water content.



Figure S16. UV-vis absorption spectra of [Eu(*pp*-dbm-Cl2)3phen] in THF/water mixture with different water content, 10 μM.



Figure S17. UV-vis absorption spectrum of [Eu(*pp*-dbm-Cl2)3phen] solid.



Figure S18. Photoluminescence spectra of [Eu(*pp*-dbm-Cl2)3phen] in THF/water mixture at different water content (*f*w), Measurement condition: *λ*ex = 360 nm, slit = 1.0–0.3, longpass filter = 380 nm.



Figure S19. Excitation spectrum of [Eu(*pp*-dbm-Cl2)3phen] solid. Measurement condition: *λ*em = 613 nm, slit = 0.5–0.1, longpass filter = 380 nm.



Figure S20. Excitation spectrum of [Eu(*mm*-dbm-Cl2)3phen] solid. Measurement condition: *λ*em = 613 nm, slit = 0.5–0.1, longpass filter = 380 nm.