# Support information for

# Efficient dye degradation and THz spectra of {$PMo_{12}$} based rare earth phosphine oxide complexes

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**Caption of Figure**

**Caption of Table**

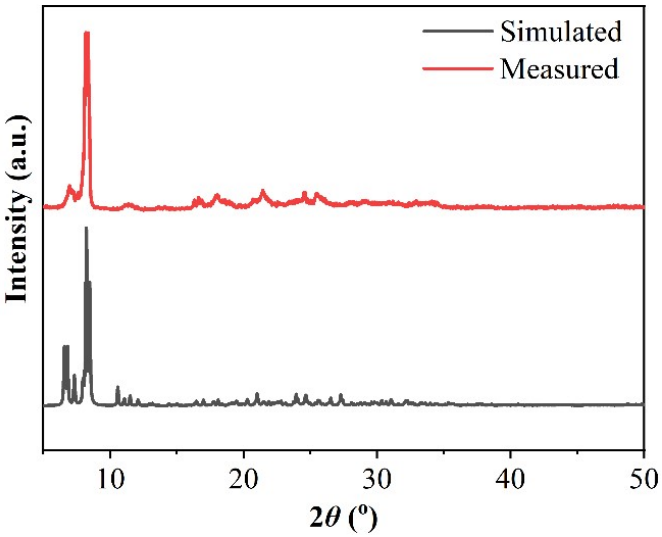


Fig S1. Powder X-ray diffraction of complex **1**

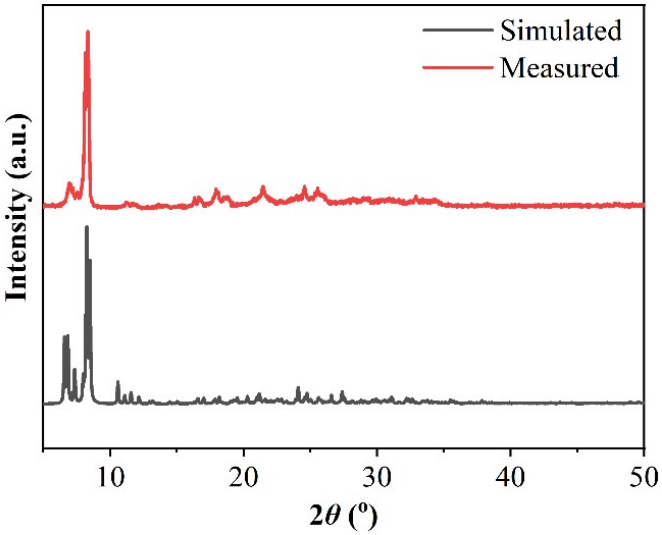


Fig S2. Powder X-ray diffraction of complex **2**

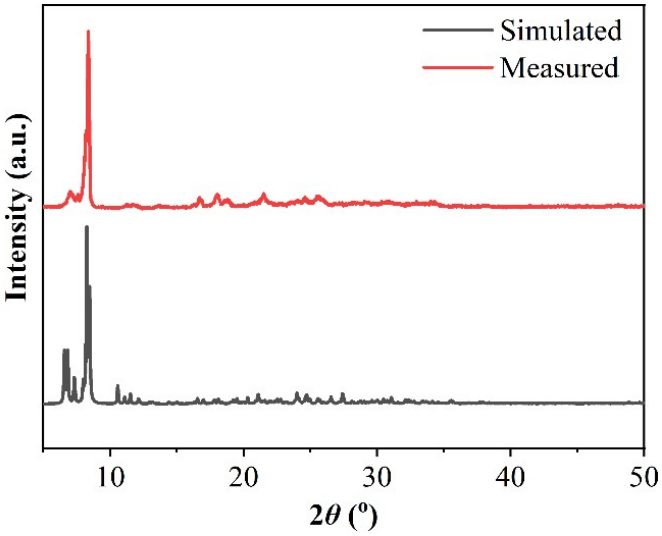


Fig S3. Powder X-ray diffraction of complex **3**

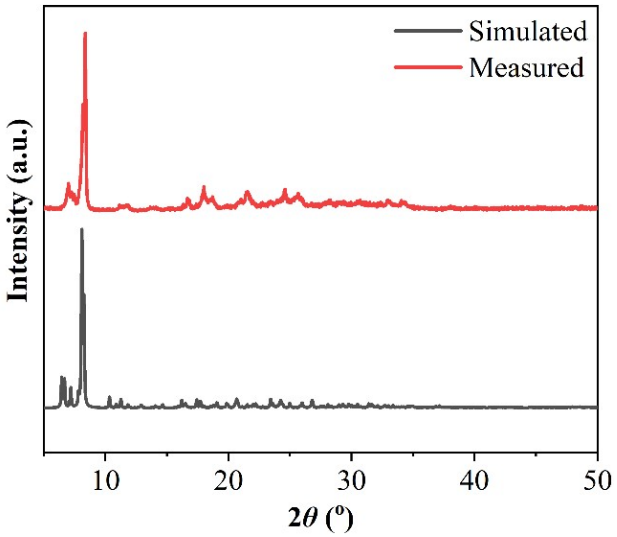


Fig S4. Powder X-ray diffraction of complex **4**

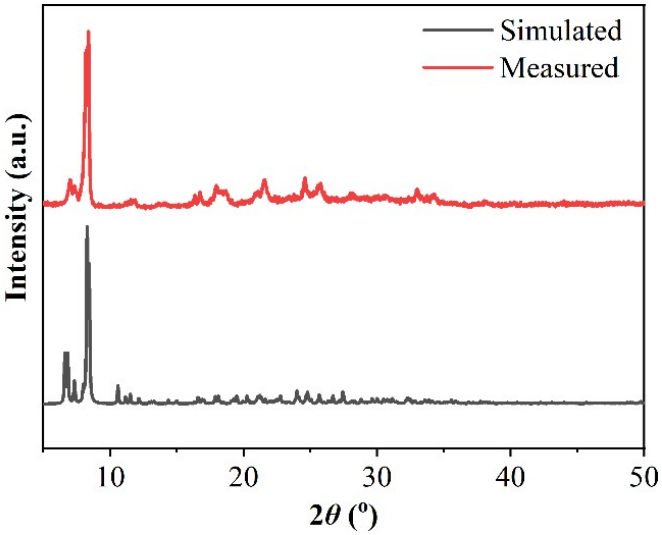


Fig S5. Powder X-ray diffraction of complex **5**

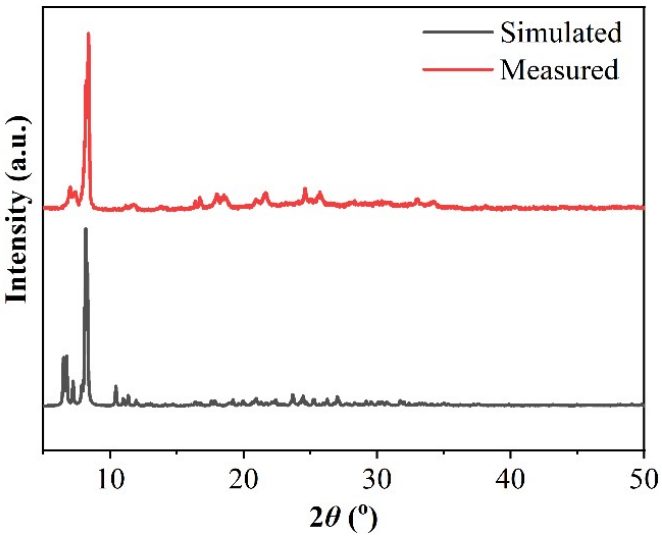


Fig S6. Powder X-ray diffraction of complex **6**

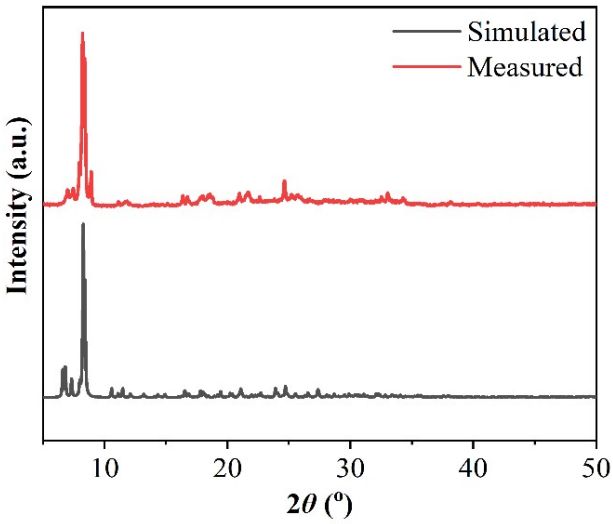


Fig S7. Powder X-ray diffraction of complex **7**

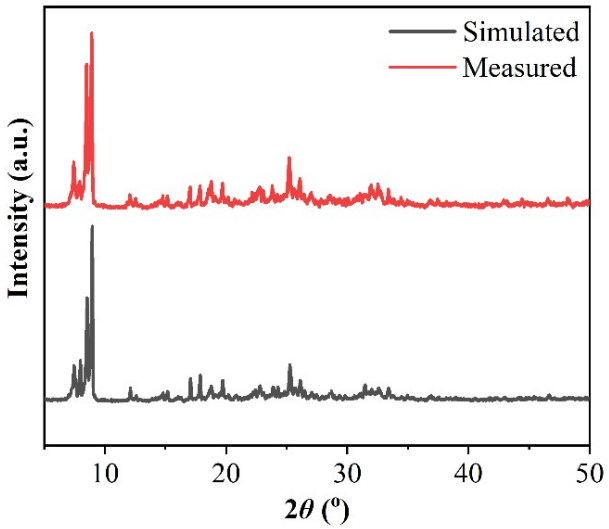


Fig S8. Powder X-ray diffraction of complex **8**

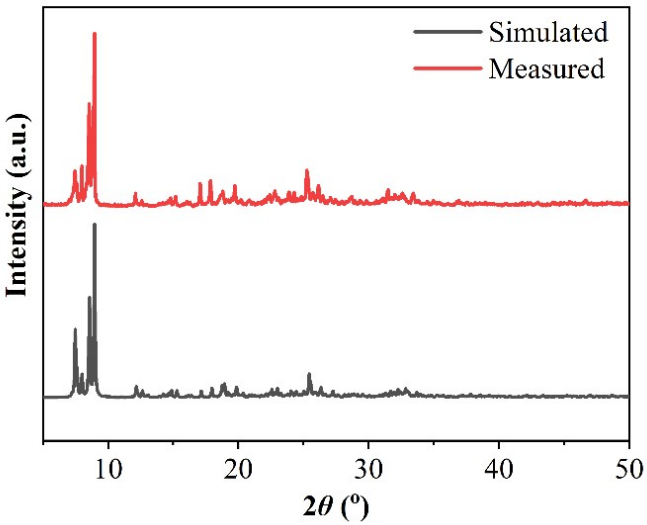


Fig S9. Powder X-ray diffraction of complex **9**

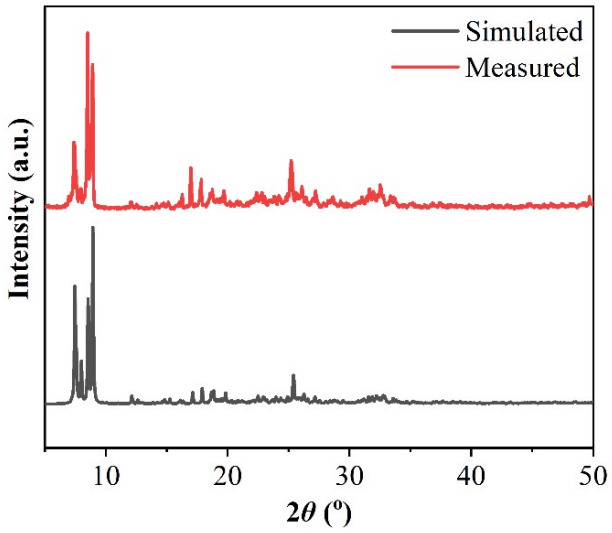


Fig S10. Powder X-ray diffraction of complex **10**

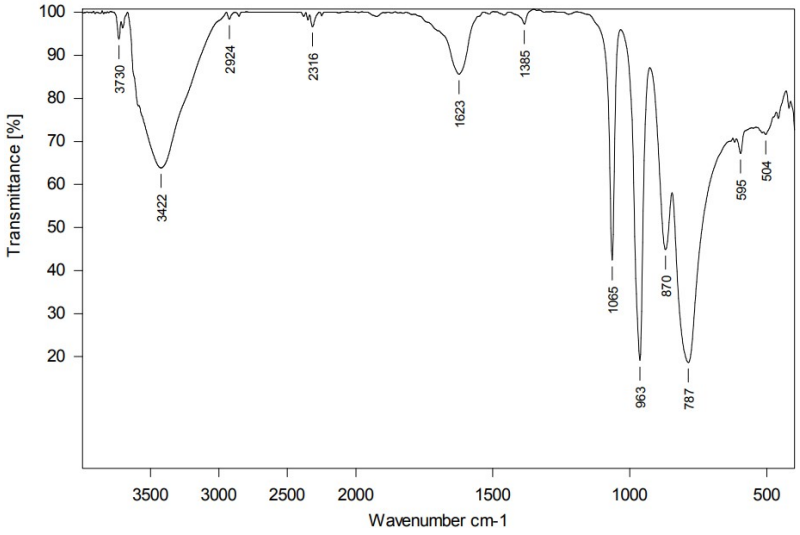


Fig. S11. The IR spectra for $H_3PMo_{12}O_{40}$

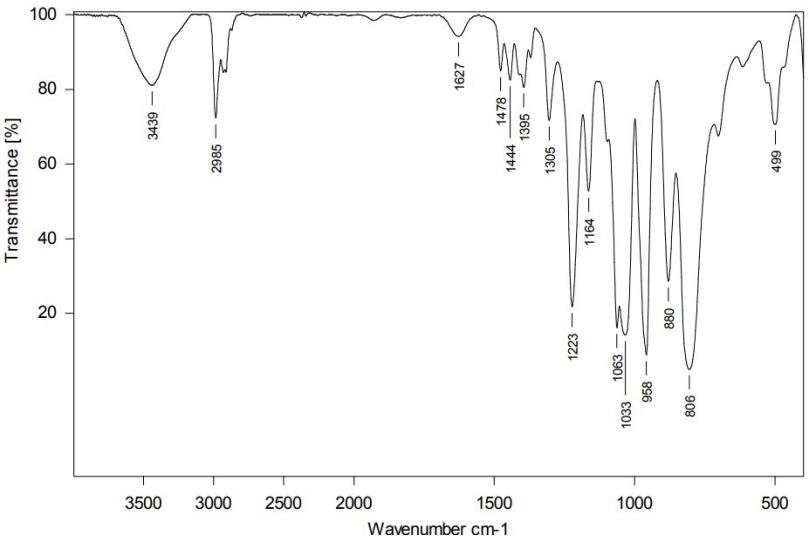


Fig. S12. The IR spectra for complex **1**

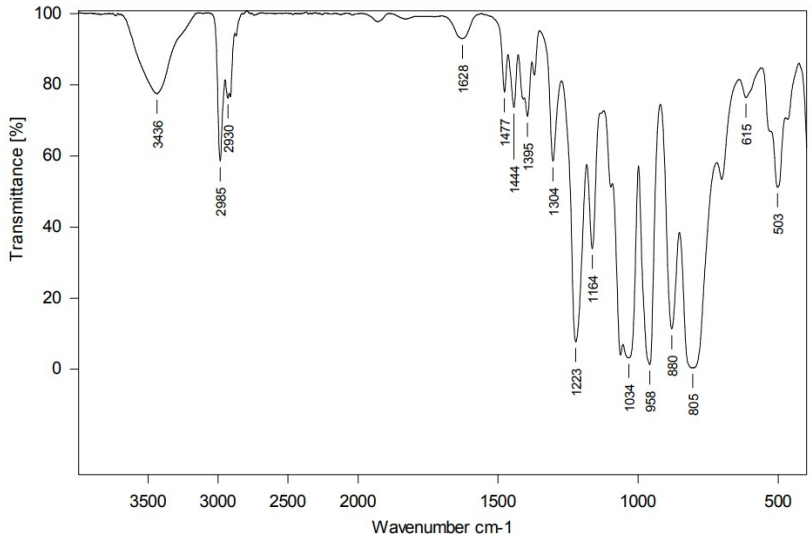


Fig. S13. The IR spectra for complex **2**

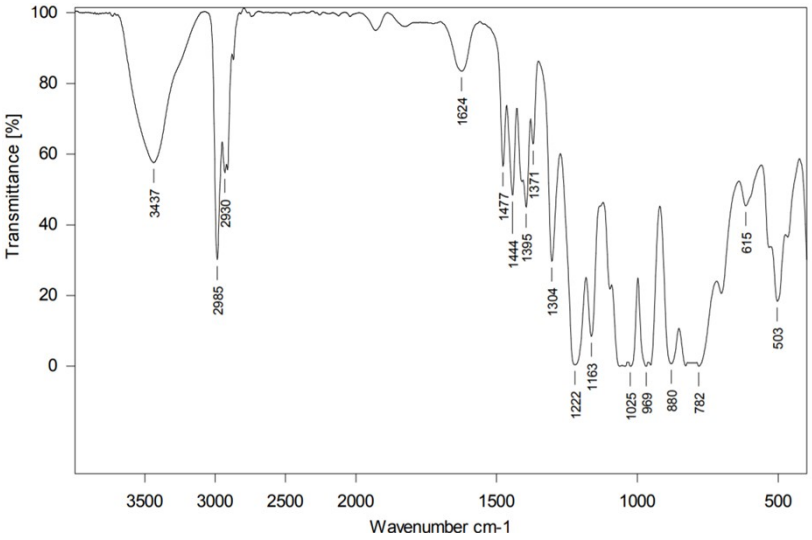


Fig. S14. The IR spectra for complex **3**

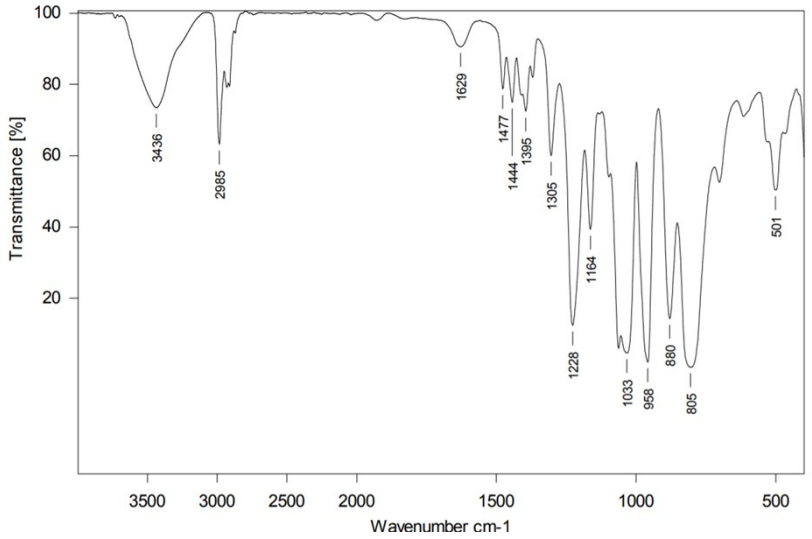


Fig. S15. The IR spectra for complex **4**

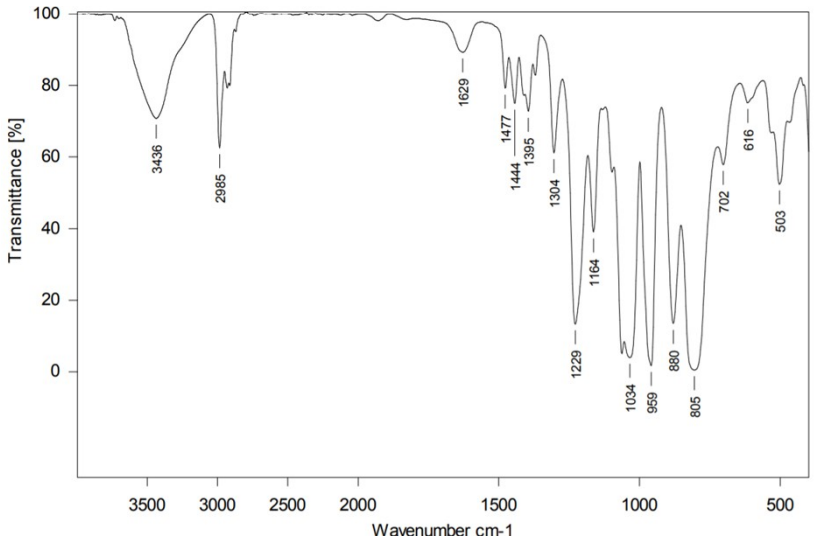


Fig. S16. The IR spectra for complex **5**

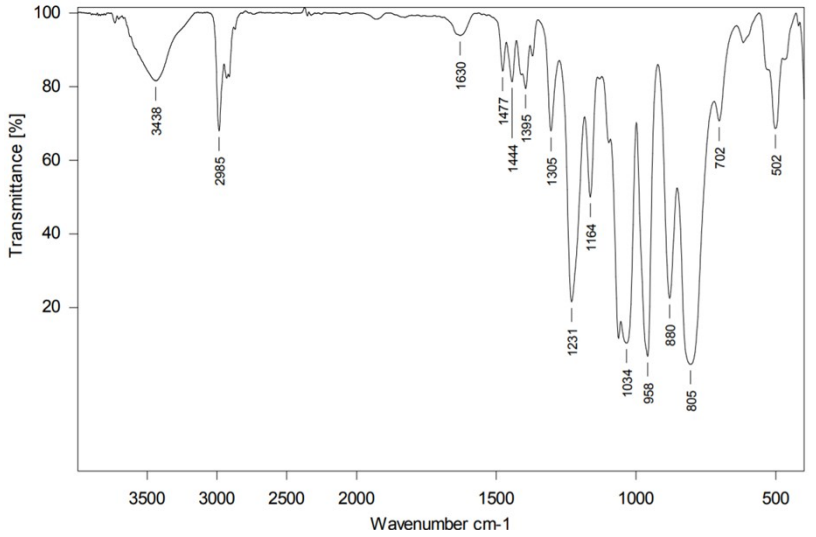


Fig. S17. The IR spectra for complex **6**

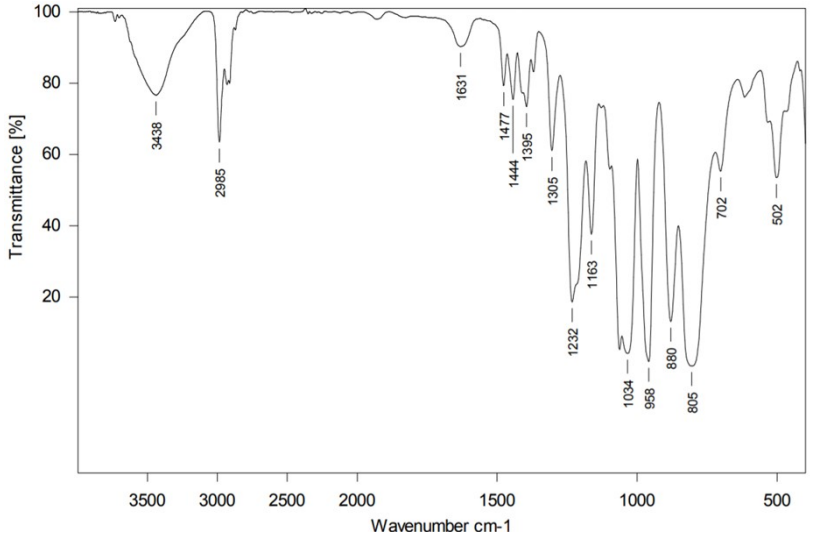


Fig. S18. The IR spectra for complex **7**

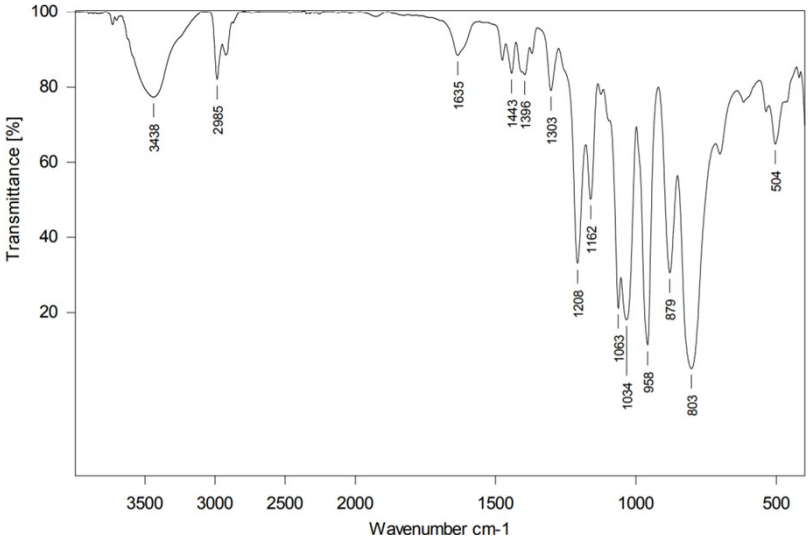


Fig. S19. The IR spectra for complex **8**

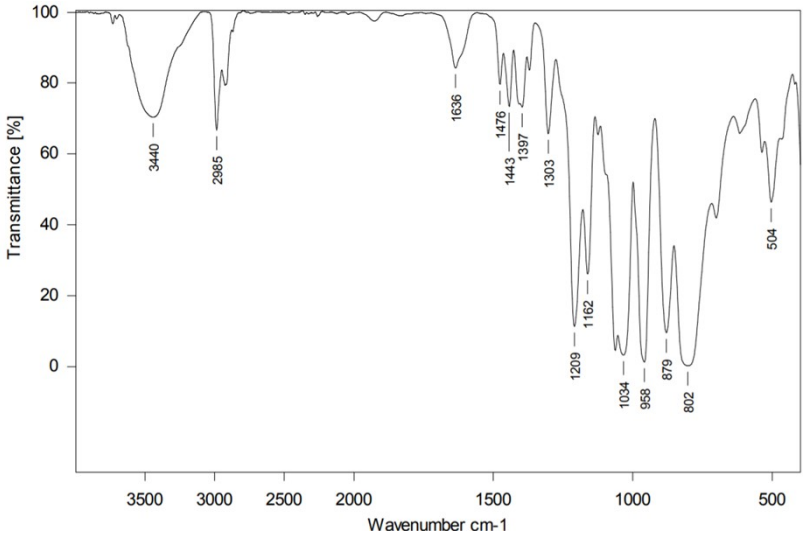


Fig. S20. The IR spectra for complex **9**

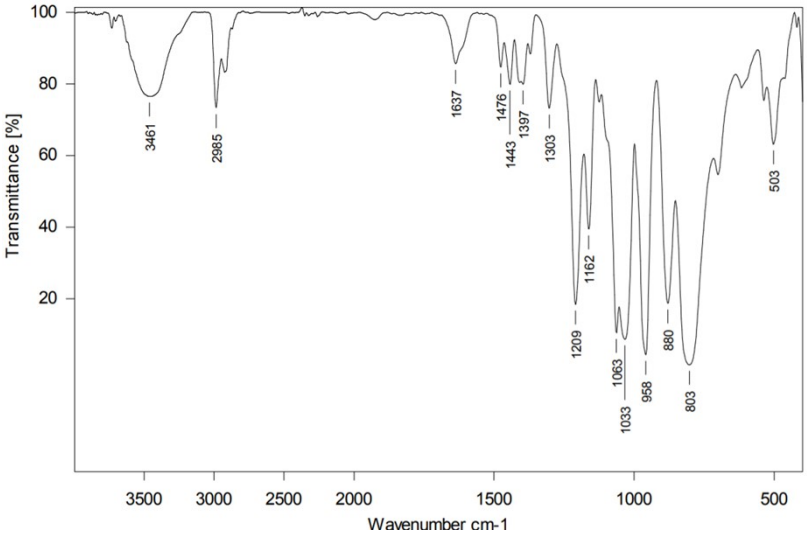


Fig. S21. The IR spectra for complex **10**

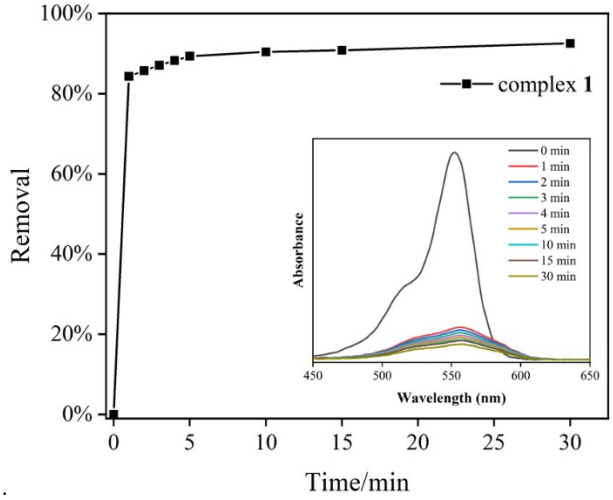


Fig. S22. Adsorption efficiency of RhB at different time intervals by complex **1**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

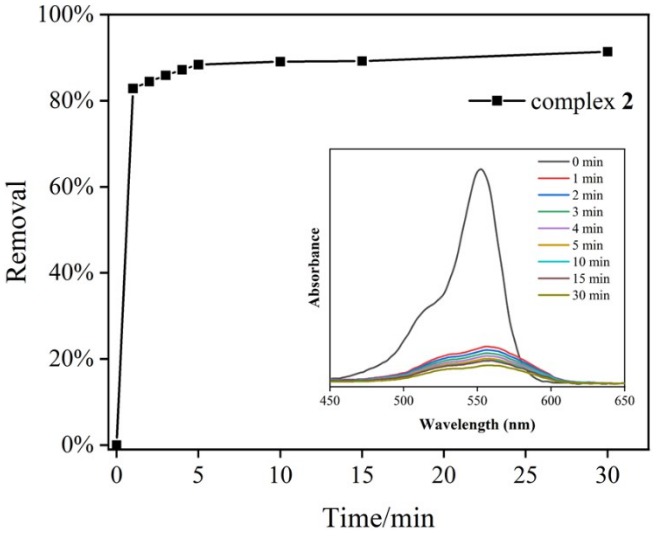


Fig. S23. Adsorption efficiency of RhB at different time intervals by complex **2**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

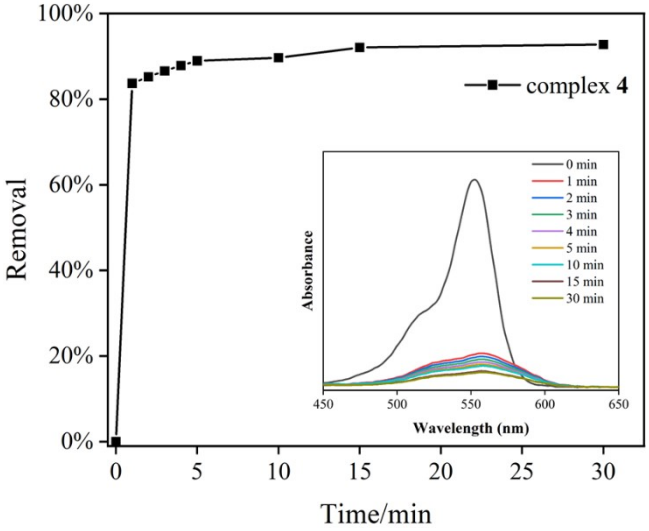


Fig. S24. Adsorption efficiency of RhB at different time intervals by complex **4**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

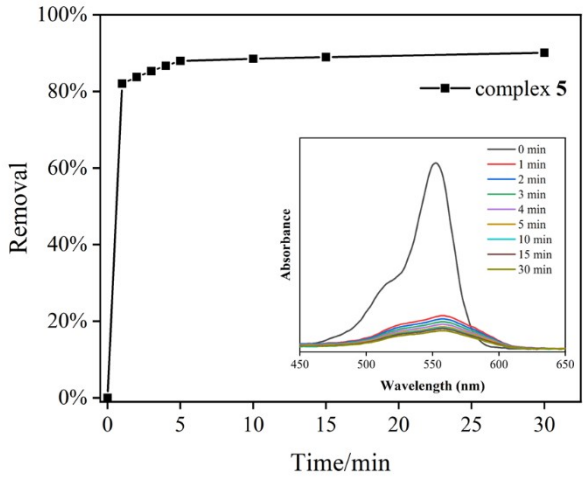


Fig. S25. Adsorption efficiency of RhB at different time intervals by complex **5**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

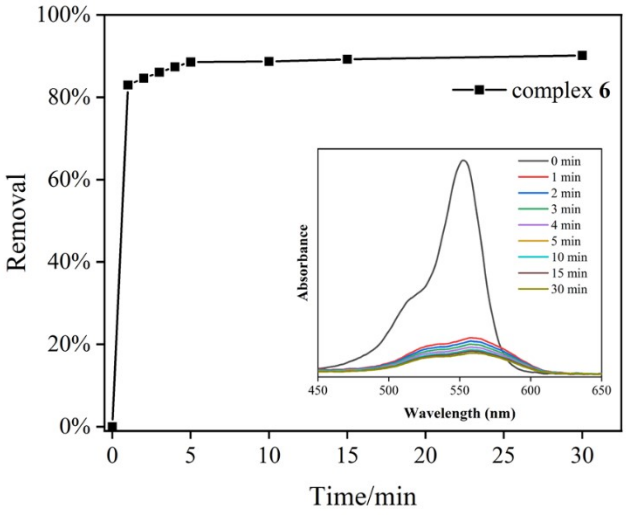


Fig. S26. Adsorption efficiency of RhB at different time intervals by complex **6**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

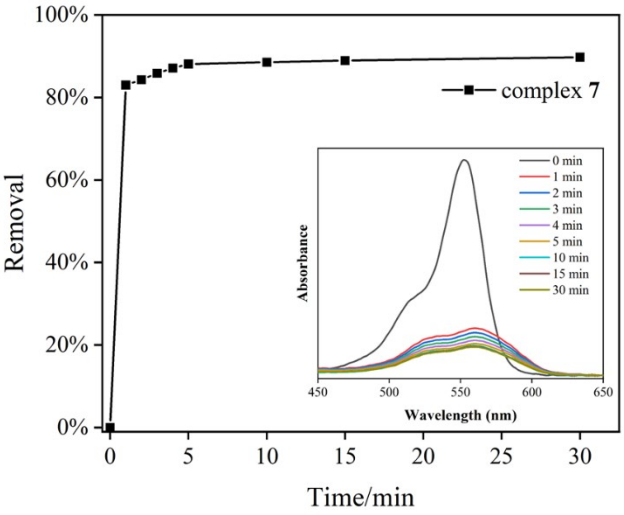


Fig. S27. Adsorption efficiency of RhB at different time intervals by complex **7**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

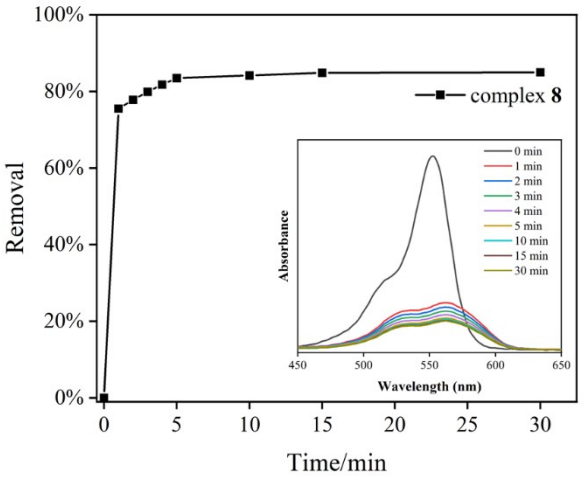


Fig. S28. Adsorption efficiency of RhB at different time intervals by complex **8**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

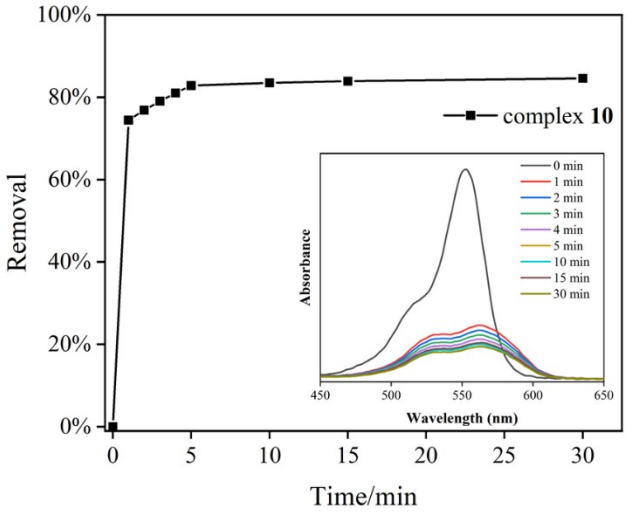


Fig. S29. Adsorption efficiency of RhB at different time intervals by complex **10**. (inset: Typical absorption spectra of RhB solution at different time intervals.)

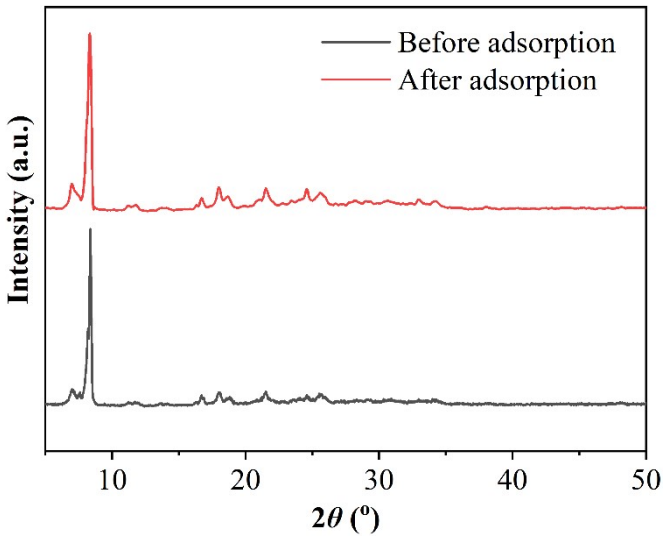


Fig. S30. PXRD of complex **3** before and after adsorption experiments.

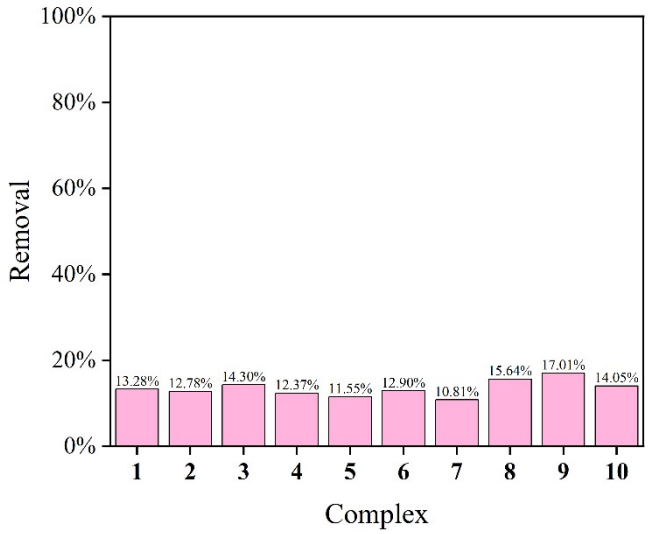


Fig. S31. Adsorption effect of MB by complexes **1-10** after stirring for 30 minutes in the dark.

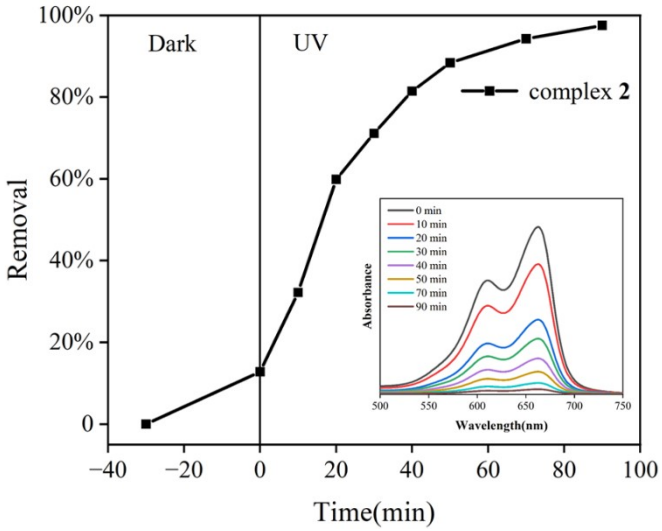


Fig. S32. Removal efficiency of MB in the photocatalytic experiment by complex **2**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

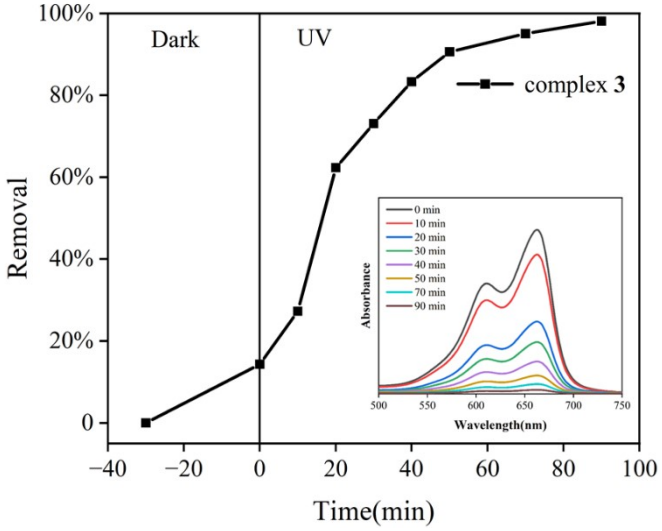


Fig. S33. Removal efficiency of MB in the photocatalytic experiment by complex **3**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

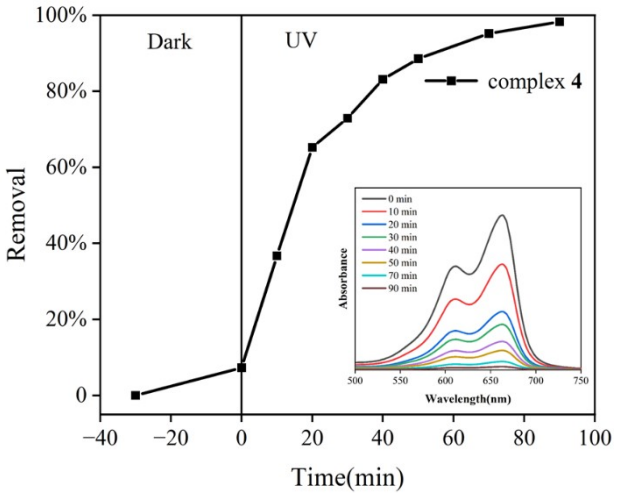


Fig. S34. Removal efficiency of MB in the photocatalytic experiment by complex **4**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

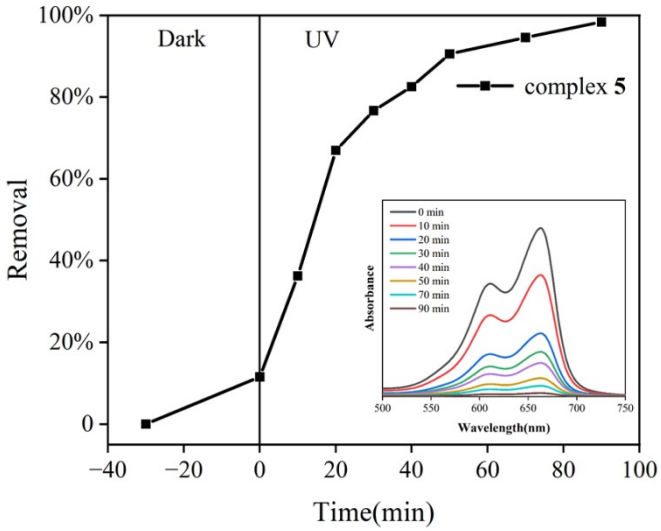


Fig. S35. Removal efficiency of MB in the photocatalytic experiment by complex **5**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

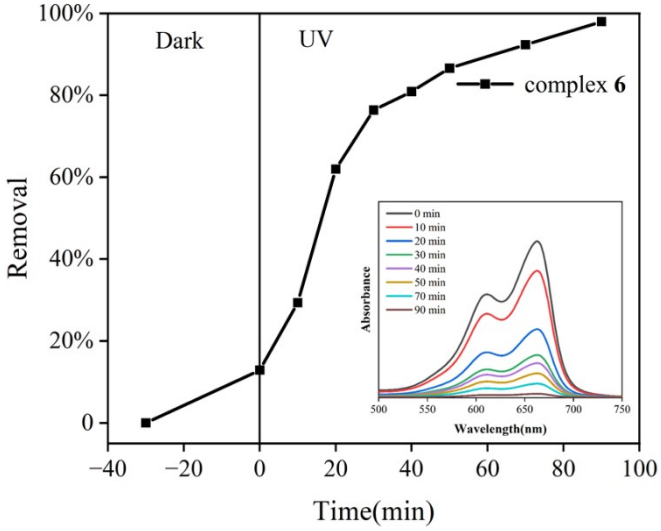


Fig. S36. Removal efficiency of MB in the photocatalytic experiment by complex **6**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

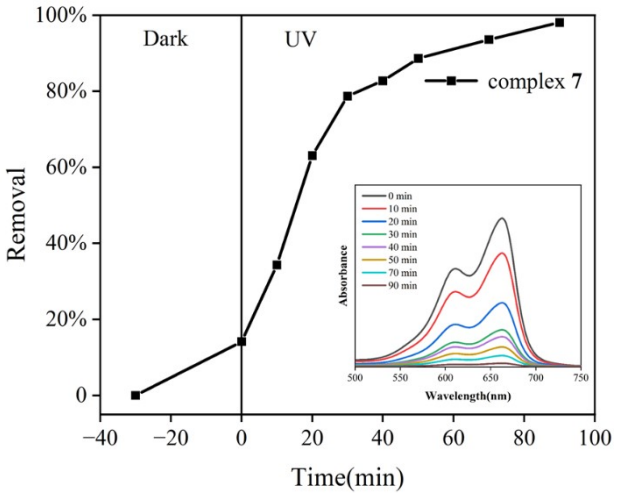


Fig. S37. Removal efficiency of MB in the photocatalytic experiment by complex **7**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

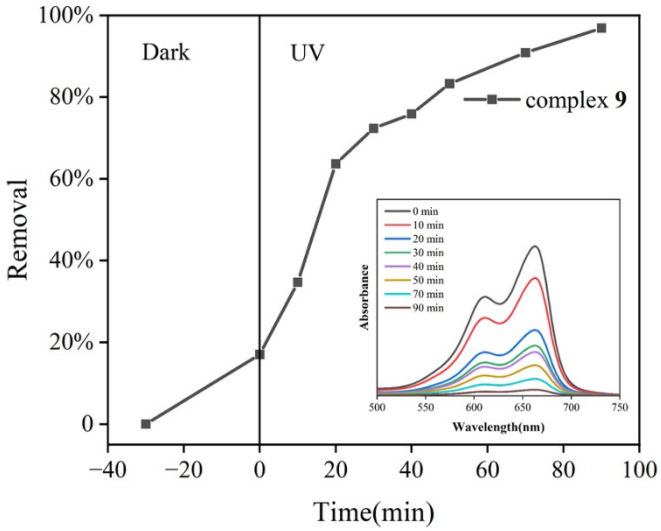


Fig. S38. Removal efficiency of MB in the photocatalytic experiment by complex **9**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

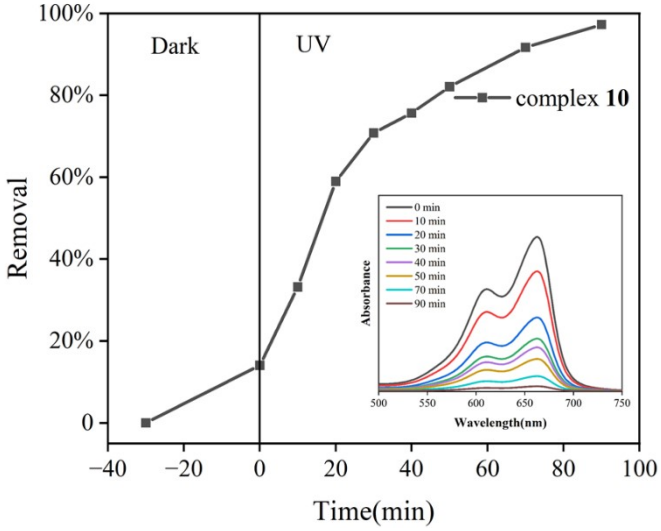


Fig. S39. Removal efficiency of MB in the photocatalytic experiment by complex **10**. (inset: UV−visible absorption spectral changes observed for the MB solution under UV light irradiation)

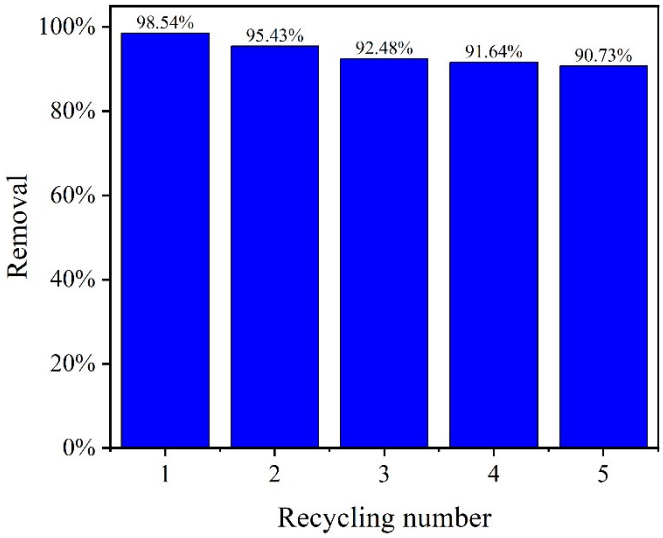


Fig. S40. The photocatalytic degradation removal rates of MB by complex **1** for 5 cycles under the same conditions

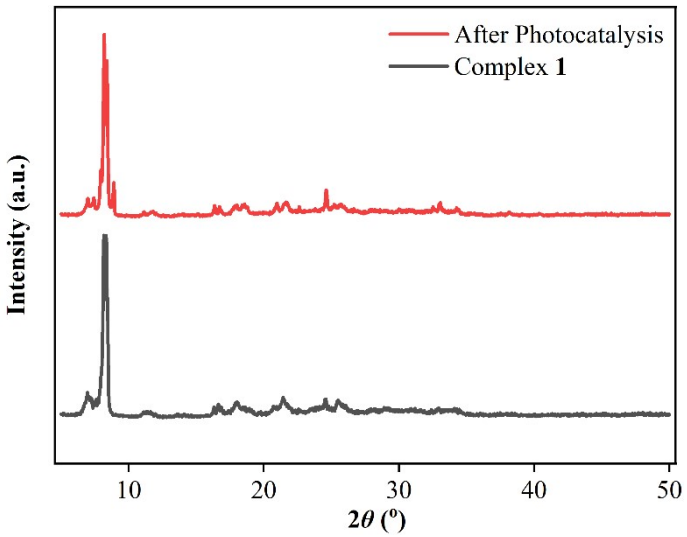


Fig. S41. PXRD of complex **1** before and after five cycles of photocatalytic experiment

Table S1. Selected bond lengths(Å) and bond angles(°) for complexes **1-10**

| **1** | | | | | |
|---|---|---|---|---|---|
| La(1)-O(45) | 2.460(13) | La(1)-O(46) | 2.463(11) | La(1)-O(47) | 2.470(10) |
| La(1)-O(48) | 2.498(13) | La(1)-O(49) | 2.436(11) | La(1)-O(50) | 2.453(11) |
| La(1)-O(51) | 2.427(12) | La(1)-O(52) | 2.492(11) | | |
| O(45)-La(1)-O(46) | 77.2(4) | O(45)-La(1)-O(47) | 72.4(5) | O(45)-La(1)-O(48) | 140.7(4) |
| O(45)-La(1)-O(49) | 113.3(4) | O(45)-La(1)-O(50) | 144.9(4) | O(45)-La(1)-O(51) | 75.4(4) |
| O(45)-La(1)-O(52) | 77.7(5) | O(46)-La(1)-O(47) | 77.5(4) | O(46)-La(1)-O(48) | 74.7(4) |
| O(46)-La(1)-O(49) | 144.0(4) | O(46)-La(1)-O(50) | 114.3(4) | O(46)-La(1)-O(51) | 142.5(4) |
| O(46)-La(1)-O(52) | 73.5(4) | O(47)-La(1)-O(48) | 75.2(4) | O(47)-La(1)-O(49) | 73.8(4) |
| O(47)-La(1)-O(50) | 141.0(4) | O(47)-La(1)-O(51) | 117.0(4) | O(47)-La(1)-O(52) | 142.0(4) |

| | | | | | |
|---|---|---|---|---|---|
| O(48)-La(1)-O(49) | 77.3(4) | O(48)-La(1)-O(50) | 73.0(4) | O(48)-La(1)-O(51) | 140.7(4) |
| O(48)-La(1)-O(52) | 118.8(4) | O(49)-La(1)-O(50) | 77.7(4) | O(49)-La(1)-O(51) | 71.7(4) |
| O(49)-La(1)-O(52) | 141.2(4) | O(50)-La(1)-O(51) | 77.2(4) | O(50)-La(1)-O(52) | 74.7(4) |
| O(51)-La(1)-O(52) | 76.0(4) | | | | |
| **2** | | | | | |
| Ce(1)-O(45) | 2.426(8) | Ce(1)-O(46) | 2.443(8) | Ce(1)-O(47) | 2.440(8) |
| Ce(1)-O(48) | 2.471(8) | Ce(1)-O(49) | 2.414(7) | Ce(1)-O(50) | 2.433(8) |
| Ce(1)-O(51) | 2.437(8) | Ce(1)-O(52) | 2.453(8) | | |
| O(45)-Ce(1)-O(46) | 77.3(3) | O(45)-Ce(1)-O(47) | 73.1(3) | O(45)-Ce(1)-O(48) | 141.3(3) |
| O(45)-Ce(1)-O(49) | 113.5(3) | O(45)-Ce(1)-O(50) | 143.9(3) | O(45)-Ce(1)-O(51) | 74.4(3) |
| O(45)-Ce(1)-O(52) | 77.3(3) | O(46)-Ce(1)-O(47) | 76.9(3) | O(46)-Ce(1)-O(48) | 74.3(3) |
| O(46)-Ce(1)-O(49) | 143.8(3) | O(46)-Ce(1)-O(50) | 114.6(3) | O(46)-Ce(1)-O(51) | 142.0(3) |
| O(46)-Ce(1)-O(52) | 74.0(3) | O(47)-Ce(1)-O(48) | 75.3(3) | O(47)-Ce(1)-O(49) | 74.0(3) |
| O(47)-Ce(1)-O(50) | 141.3(3) | O(47)-Ce(1)-O(51) | 117.3(3) | O(47)-Ce(1)-O(52) | 142.2(3) |
| O(48)-Ce(1)-O(49) | 77.8(3) | O(48)-Ce(1)-O(50) | 73.2(3) | O(48)-Ce(1)-O(51) | 141.6(3) |
| O(48)-Ce(1)-O(52) | 118.3(3) | O(49)-Ce(1)-O(50) | 77.8(3) | O(49)-Ce(1)-O(51) | 72.2(3) |
| O(49)-Ce(1)-O(52) | 140.8(3) | O(50)-Ce(1)-O(51) | 77.4(3) | O(50)-Ce(1)-O(52) | 74.1(3) |
| O(51)-Ce(1)-O(52) | 75.4(3) | | | | |
| **3** | | | | | |
| Pr(1)-O(45) | 2.417(14) | Pr(1)-O(46) | 2.426(12) | Pr(1)-O(47) | 2.392(12) |
| Pr(1)-O(48) | 2.468(14) | Pr(1)-O(49) | 2.399(12) | Pr(1)-O(50) | 2.420(12) |
| Pr(1)-O(51) | 2.411(13) | Pr(1)-O(52) | 2.435(13) | | |
| O(45)-Pr(1)-O(46) | 78.3(5) | O(45)-Pr(1)-O(47) | 72.6(5) | O(45)-Pr(1)-O(48) | 142.2(5) |
| O(45)-Pr(1)-O(49) | 113.4(5) | O(45)-Pr(1)-O(50) | 142.7(5) | O(45)-Pr(1)-O(51) | 74.7(5) |
| O(45)-Pr(1)-O(52) | 77.6(5) | O(46)-Pr(1)-O(47) | 78.0(5) | O(46)-Pr(1)-O(48) | 74.1(4) |
| O(46)-Pr(1)-O(49) | 144.0(5) | O(46)-Pr(1)-O(50) | 113.8(5) | O(46)-Pr(1)-O(51) | 143.7(5) |
| O(46)-Pr(1)-O(52) | 72.8(5) | O(47)-Pr(1)-O(48) | 76.7(4) | O(47)-Pr(1)-O(49) | 74.0(4) |
| O(47)-Pr(1)-O(50) | 142.7(5) | O(47)-Pr(1)-O(51) | 115.5(5) | O(47)-Pr(1)-O(52) | 141.8(5) |
| O(48)-Pr(1)-O(49) | 77.8(5) | O(48)-Pr(1)-O(50) | 73.4(4) | O(48)-Pr(1)-O(51) | 140.1(4) |
| O(48)-Pr(1)-O(52) | 117.0(5) | O(49)-Pr(1)-O(50) | 78.3(4) | O(49)-Pr(1)-O(51) | 70.5(5) |
| O(49)-Pr(1)-O(52) | 141.5(5) | O(50)-Pr(1)-O(51) | 76.8(5) | O(50)-Pr(1)-O(52) | 73.3(5) |
| O(51)-Pr(1)-O(52) | 78.0(5) | | | | |
| **4** | | | | | |
| Sm(1)-O(23) | 2.516(15) | Sm(1)-O(23') | 2.516(15) | Sm(1)-O(24) | 2.452(27) |
| Sm(1)-O(24') | 2.452(27) | Sm(1)-O(25) | 2.398(18) | Sm(1)-O(25') | 2.398(18) |

| | | | | | |
|---|---|---|---|---|---|
| Sm(1)-O(26) | 2.336(17) | Sm(1)-O(26′) | 2.336(17) | | |
| O(23)-Sm(1)-O(23′) | 78.3(8) | O(23)-Sm(1)-O(24) | 72.6(8) | O(23)-Sm(1)-O(24′) | 142.2(8) |
| O(23)-Sm(1)-O(25) | 113.4(8) | O(23)-Sm(1)-O(25′) | 142.7(8) | O(23)-Sm(1)-O(26) | 74.7(8) |
| O(23)-Sm(1)-O(26′) | 77.6(8) | O(23′)-Sm(1)-O(24) | 78.0(8) | O(23′)-Sm(1)-O(24′) | 74.1(8) |
| O(23′)-Sm(1)-O(25) | 144.0(8) | O(23′)-Sm(1)-O(25′) | 113.8(8) | O(23′)-Sm(1)-O(26) | 143.7(8) |
| O(23′)-Sm(1)-O(26′) | 72.8(8) | O(24)-Sm(1)-O(24′) | 76.7(8 | O(24)-Sm(1)-O(25) | 74.0(4) |
| O(24)-Sm(1)-O(25′) | 142.7(8) | O(24)-Sm(1)-O(26) | 115.5(8) | O(24)-Sm(1)-O(26′) | 141.8(8) |
| O(24′)-Sm(1)-O(25) | 77.8(8) | O(24′)-Sm(1)-O(25′) | 73.4(8 | O(24′)-Sm(1)-O(26) | 140.1(7) |
| O(24′)-Sm(1)-O(26′) | 117.0(8) | O(25)-Sm(1)-O(25′) | 78.3(8) | O(25)-Sm(1)-O(26) | 70.5(8) |
| O(25)-Sm(1)-O(26′) | 141.5(8) | O(25′)-Sm(1)-O(26) | 76.8(8) | O(25′)-Sm(1)-O(26′) | 73.3(8) |
| O(26)-Sm(1)-O(26′) | 78.0(8) | | | | |
| **5** | | | | | |
| Eu(1)-O(1) | 2.374(9) | Eu(1)-O(4) | 2.354(8) | Eu(1)-O(7) | 2.353(8) |
| Eu(1)-O(10) | 2.337(8) | Eu(1)-O(13) | 2.368(9) | Eu(1)-O(16) | 2.345(8) |
| Eu(1)-O(19) | 2.364(9) | Eu(1)-O(22) | 2.388(9) | | |
| O(1)-Eu(1)-O(4) | 77.1(3) | O(1)-Eu(1)-O(7) | 73.6(3) | O(1)-Eu(1)-O(10) | 142.1(3) |
| O(1)-Eu(1)-O(13) | 73.3(3) | O(1)-Eu(1)-O(16) | 77.9(4) | O(1)-Eu(1)-O(19) | 141.7(4) |
| O(1)-Eu(1)-O(22) | 116.5(3) | O(4)-Eu(1)-O(7) | 78.0(4) | O(4)-Eu(1)-O(10) | 72.3(3) |
| O(4)-Eu(1)-O(13) | 142.7(3) | O(4)-Eu(1)-O(16) | 73.4(3) | O(4)-Eu(1)-O(19) | 116.4(3) |
| O(4)-Eu(1)-O(22) | 141.6(3) | O(7)-Eu(1)-O(10) | 78.6(3) | O(7)-Eu(1)-O(13) | 113.9(3) |
| O(7)-Eu(1)-O(16) | 143.3(4) | O(7)-Eu(1)-O(19) | 142.0(3) | O(7)-Eu(1)-O(22) | 72.8(3) |
| O(10)-Eu(1)-O(13) | 143.0(4) | O(10)-Eu(1)-O(16) | 113.0(4) | O(10)-Eu(1)-O(19) | 73.7(3) |
| O(10)-Eu(1)-O(22) | 78.0(3) | O(13)-Eu(1)-O(16) | 78.5(3) | O(13)-Eu(1)-O(19) | 77.0(3) |
| O(13)-Eu(1)-O(22) | 73.5(3) | O(16)-Eu(1)-O(19) | 73.0(3) | O(16)-Eu(1)-O(22) | 142.2(3) |
| O(19)-Eu(1)-O(22) | 76.4(3) | | | | |
| **6** | | | | | |
| Gd(1)-O(45) | 2.390(12) | Gd(1)-O(46) | 2.371(11) | Gd(1)-O(47) | 2.403(10) |
| Gd(1)-O(48) | 2.441(12) | Gd(1)-O(49) | 2.362(12) | Gd(1)-O(50) | 2.396(11) |
| Gd(1)-O(51) | 2.394(12) | Gd(1)-O(52) | 2.410(11) | | |
| O(45)-Gd(1)-O(46) | 79.4(4) | O(45)-Gd(1)-O(47) | 72.2(5) | O(45)-Gd(1)-O(48) | 142.6(4) |
| O(45)-Gd(1)-O(49) | 112.3(5) | O(45)-Gd(1)-O(50) | 142.9(5) | O(45)-Gd(1)-O(51) | 73.1(5) |
| O(45)-Gd(1)-O(52) | 78.6(5) | O(46)-Gd(1)-O(47) | 77.0(4) | O(46)-Gd(1)-O(48) | 73.4(4) |
| O(46)-Gd(1)-O(49) | 143.1(4) | O(46)-Gd(1)-O(50) | 113.6(4) | O(46)-Gd(1)-O(51) | 143.1(4) |
| O(46)-Gd(1)-O(52) | 73.3(4) | O(47)-Gd(1)-O(48) | 76.9(4) | O(47)-Gd(1)-O(49) | 74.1(4) |
| O(47)-Gd(1)-O(50) | 143.0(4) | O(47)-Gd(1)-O(51) | 115.9(4) | O(47)-Gd(1)-O(52) | 141.5(5) |

| | | | | | |
|---|---|---|---|---|---|
| O(48)-Gd(1)-O(49) | 78.0(4) | O(48)-Gd(1)-O(50) | 73.1(4) | O(48)-Gd(1)-O(51) | 141.4(4) |
| O(48)-Gd(1)-O(52) | 116.2(5) | O(49)-Gd(1)-O(50) | 78.9(4) | O(49)-Gd(1)-O(51) | 71.8(4) |
| O(49)-Gd(1)-O(52) | 142.0(4) | O(50)-Gd(1)-O(51) | 77.9(5) | O(50)-Gd(1)-O(52) | 73.0(4) |
| O(51)-Gd(1)-O(52) | 77.6(4) | | | | |
| **7** | | | | | |
| Tb(1)-O(23) | 2.351(17) | Tb(1)-O(23′) | 2.351(17) | Tb(1)-O(24) | 2.308(17) |
| Tb(1)-O(24′) | 2.308(17) | Tb(1)-O(25) | 2.309(15) | Tb(1)-O(25′) | 2.309(15) |
| Tb(1)-O(26) | 2.254(15) | Tb(1)-O(26′) | 2.254(15) | | |
| O(23)-Tb(1)-O(23′) | 141.9(8) | O(23)-Tb(1)-O(24) | 77.9(8) | O(23)-Tb(1)-O(24′) | 78.4(8) |
| O(23)-Tb(1)-O(25) | 73.2(8) | O(23)-Tb(1)-O(25′) | 73.8(8) | O(23)-Tb(1)-O(26) | 72.9(8) |
| O(23)-Tb(1)-O(26′) | 77.3(8) | O(23′)-Tb(1)-O(24) | 76.4(8) | O(23′)-Tb(1)-O(24′) | 141.5(8) |
| O(23′)-Tb(1)-O(25) | 115.8(8) | O(23′)-Tb(1)-O(25′) | 142.3(8) | O(23′)-Tb(1)-O(26) | 112.4(8) |
| O(23′)-Tb(1)-O(26′) | 143.4(8) | O(24)-Tb(1)-O(24′) | 73.4(8) | O(24)-Tb(1)-O(25) | 79.0(8) |
| O(24)-Tb(1)-O(25′) | 78.5(8) | O(24)-Tb(1)-O(26) | 71.4(8) | O(24)-Tb(1)-O(26′) | 141.4(8) |
| O(24′)-Tb(1)-O(25) | 143.6(5) | O(24′)-Tb(1)-O(25′) | 114.3(8) | O(24′)-Tb(1)-O(26) | 72.9(8) |
| O(24′)-Tb(1)-O(26′) | 78.0(8) | O(25)-Tb(1)-O(25′) | 73.9(8) | O(25)-Tb(1)-O(26) | 73.5(8) |
| O(25)-Tb(1)-O(26′) | 142.9(8) | O(25′)-Tb(1)-O(26) | 141.8(8) | O(25′)-Tb(1)-O(26′) | 76.9(8) |
| O(26)-Tb(1)-O(26′) | 116.7(8) | | | | |
| **8** | | | | | |
| Tm(1)-O(45) | 2.239(10) | Tm(1)-O(48) | 2.238(10) | Tm(1)-O(51) | 2.237(11) |
| Tm(1)-O(54) | 2.238(10) | Tm(1)-O(57) | 2.230(11) | Tm(1)-O(60) | 2.216(11) |
| Tm(1)-O(63) | 2.361(11) | | | | |
| O(45)-Tm(1)-O(48) | 76.4(4) | O(45)-Tm(1)-O(51) | 81.1(4) | O(45)-Tm(1)-O(54) | 126.54(4) |
| O(45)-Tm(1)-O(57) | 146.4(4) | O(45)-Tm(1)-O(60) | 101.5(5) | O(45)-Tm(1)-O(63) | 71.0(4) |
| O(48)-Tm(1)-O(51) | 124.9(4) | O(48)-Tm(1)-O(54) | 76.9(4) | O(48)-Tm(1)-O(57) | 134.6(4) |
| O(48)-Tm(1)-O(60) | 76.9(4) | O(48)-Tm(1)-O(63) | 134.8(4) | O(51)-Tm(1)-O(54) | 77.5(4) |
| O(51)-Tm(1)-O(57) | 86.9(4) | O(51)-Tm(1)-O(60) | 157.5(4) | O(51)-Tm(1)-O(63) | 80.2(4) |
| O(54)-Tm(1)-O(57) | 80.5(4) | O(54)-Tm(1)-O(60) | 116.3(5) | O(54)-Tm(1)-O(63) | 148.3(4) |
| O(57)-Tm(1)-O(60) | 78.7(4) | O(57)-Tm(1)-O(63) | 76.0(4) | O(60)-Tm(1)-O(63) | 79.7(5) |
| **9** | | | | | |
| Yb(1)-O(45) | 2.219(10) | Yb(1)-O(48) | 2.208(11) | Yb(1)-O(51) | 2.208(11) |
| Yb(1)-O(54) | 2.216(10) | Yb(1)-O(57) | 2.224(12) | Yb(1)-O(60) | 2.198(11) |
| Yb(1)-O(63) | 2.349(12) | | | | |
| O(45)-Yb(1)-O(48) | 75.9(4) | O(45)-Yb(1)-O(51) | 80.8(4) | O(45)-Yb(1)-O(54) | 126.4(4) |
| O(45)-Yb(1)-O(57) | 146.4(4) | O(45)-Yb(1)-O(60) | 102.1(5) | O(45)-Yb(1)-O(63) | 71.1(4) |

| | | | | | |
|---|---|---|---|---|---|
| O(48)-Yb(1)-O(51) | 124.4(4) | O(48)-Yb(1)-O(54) | 77.0(4) | O(48)-Yb(1)-O(57) | 135.2(4) |
| O(48)-Yb(1)-O(60) | 77.3(4) | O(48)-Yb(1)-O(63) | 134.2(4) | O(51)-Yb(1)-O(54) | 77.7(4) |
| O(51)-Yb(1)-O(57) | 87.0(4) | O(51)-Yb(1)-O(60) | 157.7(4) | O(51)-Yb(1)-O(63) | 80.6(4) |
| O(54)-Yb(1)-O(57) | 80.5(4) | O(54)-Yb(1)-O(60) | 115.8(5) | O(54)-Yb(1)-O(63) | 148.7(4) |
| O(57)-Yb(1)-O(60) | 78.4(5) | O(57)-Yb(1)-O(63) | 76.1(4) | O(60)-Yb(1)-O(63) | 79.5(5) |
| **10** | | | | | |
| Y(1)-O(1) | 2.219(10) | Y(1)-O(4) | 2.208(11) | Y(1)-O(7) | 2.208(11) |
| Y(1)-O(10) | 2.216(10) | Y(1)-O(13) | 2.224(12) | Y(1)-O(16) | 2.198(11) |
| Y(1)-O(19) | 2.349(12) | | | | |
| O(1)-Y(1)-O(4) | 75.8(4) | O(1)-Y(1)-O(7) | 125.0(4) | O(1)-Y(1)-O(10) | 76.8(4) |
| O(1)-Y(1)-O(13) | 135.0(4) | O(1)-Y(1)-O(16) | 77.5(4) | O(1)-Y(1)-O(19) | 134.6(4) |
| O(4)-Y(1)-O(7) | 80.9(4) | O(4)-Y(1)-O(10) | 125.5(4) | O(4)-Y(1)-O(13) | 146.9(4) |
| O(4)-Y(1)-O(16) | 102.5(4) | O(4)-Y(1)-O(19) | 71.0(4) | O(7)-Y(1)-O(10) | 77.8(4) |
| O(7)-Y(1)-O(13) | 86.5(4) | O(7)-Y(1)-O(16) | 156.9(4) | O(7)-Y(1)-O(19) | 79.2(4) |
| O(10)-Y(1)-O(13) | 80.7(4) | O(10)-Y(1)-O(16) | 116.2(4) | O(10)-Y(1)-O(19) | 148.5(4) |
| O(13)-Y(1)-O(16) | 78.3(4) | O(13)-Y(1)-O(19) | 76.6(4) | O(16)-Y(1)-O(19) | 80.3(4) |

Table S2. Weak interactions in the stacking structure of complex **1**

Intermolecular hydrogen bonds in the stacking structure of complex **1**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(2)-H(2A)···O(15) | 0.97 | 2.43 | 3.30(2) |
| C(3)-H(3B)···O(14) | 0.97 | 2.57 | 3.38(3) |
| C(11)-H(11A)···O(13) | 0.97 | 2.39 | 3.21(2) |
| C(17)-H(17A)···O(5) | 0.97 | 2.48 | 3.41(3) |
| C(18)-H(18B)···O(21) | 0.96 | 2.35 | 3.27(2) |
| C(22)-H(22A)···O(37) | 0.97 | 2.54 | 3.43(3) |
| C(23)-H(23B)···O(30) | 0.97 | 2.46 | 3.31(3) |
| C(23)-H(23B)···O(44) | 0.97 | 2.56 | 3.32(3) |
| C(31)-H(31A)···O(39) | 0.97 | 2.58 | 3.47(3) |
| C(32)-H(32A)···O(44) | 0.97 | 2.27 | 3.23(3) |
| C(35)-H(35A)···O(29) | 0.97 | 2.57 | 3.26(3) |
| C(36)-H(36B)···O(34) | 0.96 | 2.58 | 3.45(3) |
| C(42)-H(42A)···O(22) | 0.96 | 2.57 | 3.49(3) |

Intramolecular hydrogen bonding in the stacking structure of complex **1**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(3)-H(3A)···O(54) | 0.97 | 2.49 | 2.90(3) |
| C(13)-H(13A)···O(58) | 0.97 | 2.58 | 3.00(2) |
| C(15)-H(15B)···O(47) | 0.97 | 2.44 | 2.78(3) |
| C(25)-H(25A)···O(49) | 0.97 | 2.36 | 2.88(3) |
| C(33)-H(33A)···O(66) | 0.97 | 2.54 | 2.97(3) |
| C(37)-H(37A)···O(52) | 0.96 | 2.39 | 2.84(3) |

Table S3. Weak interactions in the stacking structure of complex **2**

Intermolecular hydrogen bonds in the stacking structure of complex **2**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(2)-H(2A)···O(15) | 0.97 | 2.44 | 3.30(2) |
| C(3)-H(3B)···O(14) | 0.97 | 2.47 | 3.30(3) |
| C(11)-H(11A)···O(13) | 0.97 | 2.40 | 3.23(2) |
| C(17)-H(17A)···O(5) | 0.97 | 2.43 | 3.35(3) |
| C(22)-H(22A)···O(37) | 0.97 | 2.49 | 3.39(2) |
| C(23)-H(23B)···O(30) | 0.97 | 2.53 | 3.37(3) |
| C(23)-H(23B)···O(44) | 0.97 | 2.48 | 3.26(3) |
| C(29)-H(29B)···O(33) | 0.97 | 2.60 | 3.54(3) |
| C(32)-H(32A)···O(44) | 0.97 | 2.50 | 3.25(3) |
| C(36)-H(36B)···O(34) | 0.96 | 2.56 | 3.41(3) |
| C(42)-H(42A)···O(22) | 0.96 | 2.58 | 3.41(3) |

Intramolecular hydrogen bonding in the stacking structure of complex **2**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(2)-H(2B)···O(54) | 0.97 | 2.59 | 3.10(3) |
| C(13)-H(13A)···O(58) | 0.97 | 2.52 | 2.92(2) |
| C(15)-H(15B)···O(47) | 0.97 | 2.48 | 2.82(3) |
| C(17)-H(17B)···O(48) | 0.97 | 2.58 | 2.96(2) |
| C(25)-H(25A)···O(49) | 0.97 | 2.41 | 2.89(3) |
| C(33)-H(33A)···O(66) | 0.97 | 2.50 | 2.94(3) |

Table S4. Weak interactions in the stacking structure of complex **3**

Intermolecular hydrogen bonds in the stacking structure of complex **3**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|

| | | | |
|---|---|---|---|
| C(2)-H(2A)···O(15) | 0.97 | 2.48 | 3.29(3) |
| C(3)-H(3B)···O(14) | 0.98 | 2.52 | 3.32(3) |
| C(11)-H(11A)···O(13) | 0.97 | 2.43 | 3.25(3) |
| C(17)-H(17A)···O(5) | 0.97 | 2.43 | 3.35(3) |
| C(18)-H(18A)···O(22) | 0.96 | 2.54 | 3.49(3) |
| C(18)-H(18B)···O(21) | 0.96 | 2.35 | 3.28(3) |
| C(22)-H(22A)···O(37) | 0.97 | 2.47 | 3.37(3) |
| C(23)-H(23B)···O(30) | 0.97 | 2.48 | 3.30(3) |
| C(23)-H(23B)···O(44) | 0.97 | 2.53 | 3.28(3) |
| C(29)-H(29B)···O(33) | 0.97 | 2.55 | 3.51(3) |
| C(31)-H(31A)···O(39) | 0.97 | 2.54 | 3.44(3) |
| C(32)-H(32A)···O(44) | 0.97 | 2.24 | 3.20(3) |
| C(35)-H(35A)···O(29) | 0.97 | 2.58 | 3.28(3) |
| C(36)-H(36B)···O(34) | 0.97 | 2.56 | 3.40(3) |
| C(36)-H(36B)···O(36) | 0.97 | 2.55 | 3.34(3) |

Intramolecular hydrogen bonding in the stacking structure of complex **3**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(1)-H(1B)···O(68) | 0.97 | 2.57 | 3.45(3) |
| C(2)-H(2B)···O(54) | 0.97 | 2.54 | 3.11(3) |
| C(13)-H(13A)···O(58) | 0.97 | 2.53 | 2.96(3) |
| C(15)-H(15B)···O(47) | 0.97 | 2.54 | 2.88(3) |
| C(25)-H(25A)···O(49) | 0.97 | 2.38 | 2.87(3) |
| C(33)-H(33A)···O(66) | 0.97 | 2.50 | 2.91(3) |
| C(37)-H(37A)···O(52) | 0.97 | 2.44 | 2.89(3) |

Table S5. Weak interactions in the stacking structure of complex **4**

Intermolecular hydrogen bonds in the stacking structure of complex **4**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(4)-H(4A)···O(6) | 0.96 | 2.44 | 3.01(7) |
| C(7)-H(7A)···O(19) | 0.97 | 2.55 | 3.27(5) |
| C(20)-H(20C)···O(18) | 0.96 | 2.57 | 3.42(9) |

Intramolecular hydrogen bonding in the stacking structure of complex **4**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(5)-H(5A)···O(33) | 0.97 | 2.32 | 3.20(6) |

| | | | |
|---|---|---|---|
| C(5)-H(5B)···O(27) | 0.97 | 2.34 | 2.75(6) |

Table S6. Weak interactions in the stacking structure of complex **5**

Intermolecular hydrogen bonds in the stacking structure of complex **5**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(3)-H(3A)···O(43) | 0.97 | 2.53 | 3.47(2) |
| C(10)-H(10C)···O(34) | 0.97 | 2.48 | 3.31(3) |
| C(15)-H(15A)···O(33) | 0.97 | 2.57 | 3.52(2) |
| C(17)-H(17A)···O(40) | 0.97 | 2.46 | 3.30(2) |
| C(17)-H(17A)···O(43) | 0.97 | 2.59 | 3.30(3) |
| C(21)-H(21B)···O(51) | 0.97 | 2.47 | 3.30(2) |
| C(27)-H(27A)···O(68) | 0.97 | 2.51 | 3.37(3) |
| C(31)-H(31B)···O(66) | 0.97 | 2.39 | 3.22(2) |
| C(34)-H(34B)···O(59) | 0.96 | 2.60 | 3.33(2) |
| C(37)-H(37B)···O(60) | 0.97 | 2.49 | 3.38(2) |
| C(38)-H(38A)···O(67) | 0.96 | 2.56 | 3.52(3) |
| C(38)-H(38C)···O(53) | 0.96 | 2.39 | 3.29(2) |
| C(40)-H(40C)···O(37) | 0.96 | 2.50 | 3.37(2) |

Intramolecular hydrogen bonding in the stacking structure of complex **5**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(5)-H(5B)···O(1) | 0.97 | 2.52 | 2.99(4) |
| C(7)-H(7B)···O(6) | 0.97 | 2.54 | 2.99(3) |
| C(19)-H(19B)···O(10) | 0.97 | 2.49 | 2.96(3) |
| C(33)-H(33B)···O(21) | 0.97 | 2.57 | 2.97(2) |

Table S7. Weak interactions in the stacking structure of complex **6**

Intermolecular hydrogen bonds in the stacking structure of complex **6**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(2)-H(2A)···O(15) | 0.97 | 2.59 | 3.40(2) |
| C(3)-H(3B)···O(14) | 0.97 | 2.59 | 3.44(3) |
| C(11)-H(11A)···O(13) | 0.97 | 2.40 | 3.24(2) |
| C(17)-H(17A)···O(5) | 0.97 | 2.53 | 3.42(3) |
| C(18)-H(18B)···O(21) | 0.96 | 2.43 | 3.35(3) |
| C(22)-H(22A)···O(37) | 0.97 | 2.55 | 3.44(3) |

| | | | |
|---|---|---|---|
| C(23)-H(23B)···O(30) | 0.96 | 2.53 | 3.28(3) |
| C(31)-H(31A)···O(39) | 0.97 | 2.58 | 3.49(3) |
| C(32)-H(32A)···O(44) | 0.97 | 2.27 | 3.23(3) |
| C(36)-H(36B)···O(34) | 0.96 | 2.26 | 2.76(3) |
| C(42)-H(42A)···O(22) | 0.96 | 2.56 | 3.47(3) |

Intramolecular hydrogen bonding in the stacking structure of complex **6**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(3)-H(3A)···O(54) | 0.97 | 2.54 | 3.00(3) |
| C(19)-H(19B)···O(59) | 0.97 | 2.55 | 2.88(3) |
| C(25)-H(25A)···O(49) | 0.97 | 2.52 | 3.01(3) |
| C(37)-H(37A)···O(52) | 0.97 | 2.26 | 2.76(3) |

Table S8. Weak interactions in the stacking structure of complex **7**

Intermolecular hydrogen bonds in the stacking structure of complex **7**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(2)-H(2A)···O(5) | 0.97 | 2.58 | 3.38(4) |
| C(4)-H(4A)···O(6) | 0.96 | 2.21 | 2.87(7) |
| C(7)-H(7A)···O(19) | 0.97 | 2.46 | 3.28(5) |
| C(9)-H(9A)···O(13) | 0.97 | 2.20 | 2.99(6) |
| C(9)-H(9B)···O(11) | 0.97 | 2.19 | 2.90(6) |
| C(20)-H(20B)···O(18) | 0.95 | 2.13 | 2.79(10) |

Intramolecular hydrogen bonding in the stacking structure of complex **7**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(1)-H(1B)···O(30) | 0.97 | 2.60 | 3.13(5) |
| C(5)-H(5A)···O(33) | 0.96 | 2.53 | 3.34(6) |
| C(5)-H(5B)···O(27) | 0.97 | 2.42 | 2.81(6) |
| C(14)-H(14B)···O(32) | 0.96 | 2.56 | 3.25(6) |

Table S9. Weak interactions in the stacking structure of complex **8**

Intermolecular hydrogen bonds in the stacking structure of complex **8**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| O(63)-H(63C) ···N(1) | 0.83 | 2.00 | 2.81(2) |
| O(63)-H(63D) ···O(19) | 0.85 | 2.08 | 2.91(2) |

| | | | |
|---|---|---|---|
| C(1)-H(1A)···O(38) | 0.97 | 2.53 | 3.31(2) |
| C(1)-H(1B)···O(14) | 0.97 | 2.46 | 3.39(2) |
| C(2)-H(2B)···O(35) | 0.97 | 2.53 | 3.37(2) |
| C(12)-H(12B)···O(31) | 0.97 | 2.58 | 3.48(2) |
| C(14)-H(14B)···O(10) | 0.96 | 2.51 | 3.46(3) |
| C(19)-H(19B)···O(31) | 0.97 | 2.51 | 3.21(2) |
| C(20)-H(20A)···O(32) | 0.96 | 2.59 | 3.42(3) |
| C(25)-H(25A)···O(34) | 0.97 | 2.50 | 3.46(3) |
| C(26)-H(26B)···O(38) | 0.97 | 2.44 | 3.44(3) |
| C(26)-H(26C)···O(16) | 0.96 | 2.56 | 3.26(3) |
| C(29)-H(29B)···O(16) | 0.97 | 2.45 | 3.41(3) |
| C(32)-H(32A)···O(12) | 0.96 | 2.49 | 3.43(2) |

Intramolecular hydrogen bonding in the stacking structure of complex **8**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(7)-H(7B)···O(56) | 0.97 | 2.52 | 3.23(2) |
| C(17)-H(17A)···O(58) | 0.97 | 2.53 | 3.45(3) |
| C(23)-H(23A)···O(59) | 0.97 | 2.51 | 2.85(3) |
| C(25)-H(25B)···O(57) | 0.97 | 2.55 | 2.95(2) |

Table S10. Weak interactions in the stacking structure of complex **9**

Intermolecular hydrogen bonds in the stacking structure of complex **9**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| O(63)-H(63C)···N(1) | 0.83 | 2.00 | 2.81(3) |
| O(63)-H(63D)···O(19) | 0.86 | 2.06 | 2.89(2) |
| C(1)-H(1A)···O(38) | 0.97 | 2.52 | 3.31(2) |
| C(1)-H(1B)···O(14) | 0.97 | 2.42 | 3.35(2) |
| C(2)-H(2B)···O(35) | 0.97 | 2.54 | 3.37(2) |
| C(12)-H(12B)···O(31) | 0.97 | 2.60 | 3.49(2) |
| C(14)-H(14B)···O(10) | 0.96 | 2.52 | 3.46(3) |
| C(19)-H(19B)···O(31) | 0.97 | 2.49 | 3.21(2) |
| C(25)-H(25A)···O(34) | 0.97 | 2.51 | 3.46(3) |
| C(26)-H(26B)···O(38) | 0.95 | 2.45 | 3.35(3) |
| C(26)-H(26C)···O(16) | 0.96 | 2.49 | 3.22(3) |
| C(29)-H(29B)···O(16) | 0.97 | 2.43 | 3.39(3) |

| | | | |
|---|---|---|---|
| C(32)-H(32A)···O(12) | 0.96 | 2.50 | 3.43(3) |

Intramolecular hydrogen bonding in the stacking structure of complex **9**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(7)-H(7B)···O(56) | 0.97 | 2.50 | 3.21(2) |
| C(17)-H(17A)···O(58) | 0.97 | 2.54 | 3.46(3) |
| C(23)-H(23A)···O(59) | 0.97 | 2.54 | 2.90(2) |
| C(25)-H(25B)···O(57) | 0.97 | 2.58 | 2.95(2) |
| C(27)-H(27A)···O(60) | 0.97 | 2.59 | 3.02(3) |

Table S11. Weak interactions in the stacking structure of complex **10**

Intermolecular hydrogen bonds in the stacking structure of complex **10**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| O(19)-H(19E)···N(1) | 0.85 | 1.98 | 2.81(2) |
| O(19)-H(19F)···O(28) | 0.85 | 2.04 | 2.87(2) |
| C(1)-H(1B)···O(58) | 0.97 | 2.54 | 3.39(2) |
| C(2)-H(2A)···O(63) | 0.97 | 2.59 | 3.36(2) |
| C(2)-H(2B)···O(36) | 0.97 | 2.42 | 3.35(2) |
| C(10)-H(10B)···O(41) | 0.96 | 2.58 | 3.46(3) |
| C(14)-H(14B)···O(30) | 0.96 | 2.58 | 3.45(3) |
| C(19)-H(19B)···O(53) | 0.97 | 2.47 | 3.22(2) |
| C(23)-H(23A)···O(57) | 0.97 | 2.58 | 2.99(2) |
| C(24)-H(24B)···O(63) | 0.96 | 2.41 | 3.36(3) |
| C(25)-H(25B)···O(41) | 0.97 | 2.56 | 3.26(2) |
| C(27)-H(27B)···O(33) | 0.97 | 2.51 | 3.44(3) |
| C(32)-H(32B)···O(33) | 0.96 | 2.52 | 3.39(3) |

Intramolecular hydrogen bonding in the stacking structure of complex **10**

| Donor-H···Acceptor | D-H (Å) | H-A (Å) | D-A (Å) |
|---|---|---|---|
| C(3)-H(3B)···O(12) | 0.97 | 2.52 | 3.23(2) |
| C(23)-H(23B)···O(13) | 0.97 | 2.58 | 2.99(2) |
| C(25)-H(25A)···O(14) | 0.97 | 2.54 | 2.88(2) |