Supporting Information

Tuning the Structure, dimensionality and Luminescent properties of Lanthanide Metal-Organic Frameworks under Ancillary Ligand Influence. †

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Supporting Information.

Section S1. Experimental X-ray powder patterns for $[Ln(3-OHNDS)(H_2O)_2, [Ln(3-OHNDS)(phen)(H_2O)] \cdot 3H_2O$ and $[La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)]$ compounds.

Section S2. TG analysis for the $[Ln(3-OHNDS)(H_2O)_2, [Ln(3-OHNDS)(phen)(H_2O)] \cdot 3H_2O$ and $[La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)]$ compounds.

Section S3. IR spectra of $[Ln(3-OHNDS)(H_2O)_2, [Ln(3-OHNDS)(phen)(H_2O)]\cdot 3H_2O$ and $[La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)]$ compounds.

Section S4. Excitation spectrum of the compounds $[Ln(3-OHNDS)(H_2O)_2where Ln = La (1), Pr(2), Nd(3) and Sm(4); and <math>[Ln(3-OHNDS)(phen)(H_2O)] \cdot 3H_2O$, where Ln = La(5), Pr(6), Nd(7) and Sm(8).

Section S5. Assignment of the transitions in the excitation and emission spectra of 3-OHNDS and compounds (1)-(8).

Section S6. Luminescence decay traces for compounds (1)-(8).

Section S7. CIE coordinates and color emission of 3-OHNDS y (1)-(8) compounds.

Section S8. Squeeze results.

Section S1. Experimental X-ray powder patterns for $[Ln(3-OHNDS)(H_2O)_2, [Ln(3-OHNDS)(phen)(H_2O)] \cdot 3H_2O$ and $[La(3-OHNDS)(3,4,7,8-TMphen)(H_2O)]$ compounds.







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Figure S4.1. Excitation spectrum of compound (1) monitored at 430 nm.



Figure S4.2. Excitation spectrum of compound (5) monitored at 430 nm.



Figure S4.3. Excitation spectrum of compound (2) monitored at 610 nm.



Figure S4.4. Excitation spectrum of compound (6) monitored at 610 nm.



Figure S4.5. Excitation spectrum of compound (3) monitored at 464 nm.



Figure S4.6. Excitation spectrum of compound (7) monitored at 464 nm.



Figure S4.7. Excitation spectrum of compound (4) monitored at 594 nm.



Figure S4.8. Excitation spectrum of compound (8) monitored at 594 nm.

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Section S5. Assignment of the transitions in the excitation and emission spectra of 3-OHNDS and compounds (1)-(8).

Table S1. Assignment of the transitions in the excitation and emission spectra of 3-OHNDS and compounds(1)-(9).

| | | | | 3-0 | HNDS | | | |
|-------|----------------|----------------------------|---|-----|-------|----------------|----------------------------|---|
| | | Excitation | | | | | Emission | |
| Label | λ (nm) | Energy (cm ⁻¹) | Transition | | Label | λ (nm) | Energy (cm ⁻¹) | Transition |
| а | 279.9 | 35727 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ | | c | 379.1 | 26378 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b | 308 | 32468 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ | | d | 415.9 | 24044 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | (1) | | | | |
| | | Excitation | | | | | Emission | |
| Label | λ (nm) | Energy (cm ⁻¹) | Transition | | Label | λ (nm) | Energy (cm ⁻¹) | Transition |
| a | 319.9 | 31260 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ | | b | 431.9 | 23154 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | Excitation | | (2) | | | Emission | |
| Label | λ (nm) | Energy (cm ⁻¹) | Transition | | Label | λ (nm) | Energy (cm ⁻¹) | Transition |
| а | 340.9 | 29334 | $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | | g | 449.1 | 22267 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b | 351.4 | 28458 | $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | | h | 466 | 21459 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| c | 394.9 | 25323 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ | | i | 488.9 | 20454 | $^{3}P_{0}\rightarrow ^{3}H_{4}$ |
| d | 476.65 | 20980 | ${}^{3}P_{1} \leftarrow {}^{3}H_{4}$ | | j | 502.4 | 19904 | $^{3}P_{0} \rightarrow ^{3}H_{5}$ |
| e | 494.9 | 20206 | $^{3}P_{0} \leftarrow ^{3}H_{4}$ | | k | 529.1 | 18900 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| f | 520.9 | 19198 | not assignable | | 1 | 586.4 | 17053 | $^{1}D_{2} \rightarrow ^{3}H_{4}$ |
| | | | | | m | 611.8 | 16345 | ${}^{3}P_{0} \rightarrow {}^{3}H_{6}$ |
| | | | | | n | 634.3 | 15765 | ${}^{3}P_{0} \rightarrow {}^{3}F_{2}$ |
| | | | | | 0 | 684.4 | 14611 | $^{1}D_{2}\rightarrow ^{3}H_{5}$ |
| | | | | | р | 711 | 14065 | ${}^{3}P_{0} \rightarrow {}^{3}F_{3}$ |
| | | | | | | 728 | 13736 | |
| | | | | (3) | | | | |
| | | Excitation | | | | | Emission | |
| Label | λ (nm) | Energy (cm ⁻¹) | Transition | | Label | λ (nm) | Energy (cm ⁻¹) | Transition |
| a | 280.9 | 35600 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ | | b | 410.7 | 24349 | $^{2}P_{3/2} {\longrightarrow} ^{4}I_{9/2}$ |
| | | | | | c | 435.9 | 22941 | ${}^2P_{3/2} {\longrightarrow} {}^4I_{11/2}$ |
| | | | | | d | 447.9 | 22326 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | e | 464.9 | 21510 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | f | 479.3 | 20864 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | g | 488.4 | 20475 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | h | 507.3 | 19712 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |

| | | | | | i | 533.8 | 18734 | $^{2}G_{7/2}\!\!+^{4}G_{5/2}\!\!\rightarrow^{4}\!I_{9/2}$ |
|--|---|---|--|--------------|---|---|---|--|
| | | | | | j | 559.8 | 17864 | $^2G_{7/2}\text{+}{}^4G_{5/2} \text{\longrightarrow} {}^4I_{9/2}$ |
| | | | | | k | 569.3 | 17565 | $^{2}G_{7/2}\text{+}^{4}G_{5/2} \text{\longrightarrow} ^{4}I_{9/2}$ |
| | | | | | 1 | 584.6 | 17106 | ${}^{2}G_{7/2} + {}^{4}G_{5/2} \rightarrow {}^{4}I_{9/2}$ |
| | | | | (4) | | | | |
| | | Excitation | | | | | Emission | |
| Label | λ (nm) | Energy (cm ⁻¹) | Transition | | Label | λ (nm) | Energy (cm ⁻¹) | Transition |
| a | 329.6 | 30340 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ | | i | 449.6 | 22242 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b | 380.6 | 26274 | $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | | j | 464.2 | 21542 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| c | 434.9 | 22994 | ⁴ G _{9/2} ← ⁶ H _{5/2} | | k | 483.7 | 20674 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| d | 450.9 | 22178 | ${}^{4}M_{17/2}, {}^{4}F_{5/2} \leftarrow {}^{6}H_{5/2}$ | | 1 | 496.4 | 20145 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| e | 466.6 | 21432 | ${}^{4}I_{13/2} \leftarrow {}^{6}H_{5/2}$ | | m | 530.7 | 18843 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| f | 483.4 | 20687 | ${}^{4}\mathrm{I}_{11/2}, {}^{4}\mathrm{M}_{15/2} {\leftarrow} {}^{6}\mathrm{H}_{5/2}$ | | n | 559 | 17889 | ${}^{4}G_{5/2} {\rightarrow} {}^{6}H_{5/2}$ |
| g | 494.9 | 20206 | ⁴ I _{9/2} , ⁴ G _{7/2} ← ⁶ H _{5/2} | | 0 | 593.9 | 16838 | ${}^{4}G_{5/2} \rightarrow {}^{6}H_{7/3}$ |
| h | 511.1 | 19566 | ⁴ I _{11/2} , ← ⁶ H _{5/2} | | р | 639.9 | 15627 | ${}^{4}G_{5/2} \rightarrow {}^{6}H_{9/4}$ |
| | | | | | q | 687.8 | 14539 | ${}^{4}G_{5/2} \rightarrow {}^{6}H_{11/5}$ |
| | | | | | r | 708.6 | 14112 | ${}^{4}G_{5/2} \rightarrow {}^{6}H_{11/5}$ |
| | | | | (5) | | | | |
| | | Excitation | | | | | Emission | |
| | | | | | | | | |
| Label | λ (nm) | Energy (cm ⁻¹) | Transition | | Label | λ (nm) | Energy (cm ⁻¹) | Transition |
| Label a | λ (nm) 277.5 | Energy (cm ⁻¹) 36036 | $\frac{\text{Transition}}{\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*}$ | | Label c | λ (nm) 430.2 | Energy (cm ⁻¹) 23245 | $\frac{\text{Transition}}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ |
| Label a b | λ (nm) 277.5 306 | Energy (cm ⁻¹) 36036 32680 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | | Label c | λ (nm) 430.2 | Energy (cm ⁻¹) 23245 | $\frac{\text{Transition}}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ |
| Label a b | λ (nm) 277.5 306 | Energy (cm ⁻¹) 36036 32680 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | (6) | Label c | λ (nm) 430.2 | Energy (cm ⁻¹) 23245 Emission | $\frac{\text{Transition}}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ |
| Label a b | λ (nm) 277.5 306 | Energy (cm ⁻¹) 36036 32680 Excitation | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ Transition | (6) | Label c | λ (nm) 430.2 λ (nm) | Energy (cm ⁻¹) 23245 Emission | Transition $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ Transition |
| Label a b Label a | $\frac{\lambda \text{ (nm)}}{277.5}$ 306 $\lambda \text{ (nm)}$ 351.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | (6) | Label c Label | $\frac{\lambda \text{ (nm)}}{430.2}$ $\frac{\lambda \text{ (nm)}}{451.9}$ | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 | Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ |
| Label a b Label a b | λ (nm) 277.5 306 λ (nm) 351.4 413.6 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | (6) | Label c Label h i | $\frac{\lambda \text{ (nm)}}{430.2}$ $\frac{\lambda \text{ (nm)}}{451.9}$ 463.8 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 | Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ |
| Label a b Label a b c | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | (6) | Label c Label h i j | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 | Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ |
| Label a b Label a b c d | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi^* \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $3P_2 \leftarrow ^3H_4$ | (6) | Label c Label h i j k | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 | $\begin{array}{c} Transition \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \hline \\ \hline \\ \hline \\ \hline \\ \hline \\ \hline \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \hline \\ \pi^3 P_0 \rightarrow {}^3H_4 \end{array}$ |
| Label a Label a b c d e | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 21026 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $3P_2 \leftarrow ^3H_4$ $^3P_1 \leftarrow ^3H_4$ | (6) | Label c Label h i j k l | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 | Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ Transition $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ $3P_0 \rightarrow ^3H_4$ $\pi^* \rightarrow \pi$ or $\pi^* \rightarrow n$ |
| Label a b Label a b c d d e f | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 22104 21026 20186 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $^{3}P_{2} \leftarrow ^{3}H_{4}$ $^{3}P_{1} \leftarrow ^{3}H_{4}$ $^{3}P_{0} \leftarrow ^{3}H_{4}$ | (6) | Label c Label h i j k l m | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 16526 | $\begin{array}{c} Transition \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \hline \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ 3P_0 \rightarrow ^3H_4 \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ 3P_0 \rightarrow ^3H_6 \end{array}$ |
| Label a b Label a b c d e f g | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 520.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 22104 21026 20186 19216 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $3P_2 \leftarrow ^3H_4$ $^3P_1 \leftarrow ^3H_4$ $^3P_0 \leftarrow ^3H_4$ not assignable | (6) | Label c Label h i j k l m n | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 644.4 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 16526 15518 | $\begin{array}{c} Transition \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \hline \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ 3P_0 \rightarrow ^3H_4 \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n \\ ^3P_0 \rightarrow ^3H_6 \\ ^3P_0 \rightarrow ^3F_2 \end{array}$ |
| Label a b Label a b c d e f g | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 520.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 22104 21026 20186 19216 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $3P_2 \leftarrow ^3H_4$ $^3P_1 \leftarrow ^3H_4$ $^3P_0 \leftarrow ^3H_4$ not assignable | (6) | Label c Label h i j k 1 m n o | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 644.4 682.8 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 16526 15518 14646 | $\begin{array}{c} Transition\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \end{array}$ $\begin{array}{c} \hline \\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ 3^{P}_{0} \rightarrow {}^{3}H_{4}\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ 3^{P}_{0} \rightarrow {}^{3}H_{6}\\ 3^{P}_{0} \rightarrow {}^{3}F_{2}\\ 1^{D}_{2} \rightarrow {}^{3}H_{5} \end{array}$ |
| Label a Label a b c d e f g | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 520.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 22104 21026 20186 19216 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $3P_2 \leftarrow ^3H_4$ $^3P_1 \leftarrow ^3H_4$ $^3P_0 \leftarrow ^3H_4$ not assignable | (6) | Label c Label h i j k l m n o p | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 644.4 682.8 714 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 16526 15518 14646 14006 | $\begin{array}{c} Transition\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \end{array}$ $\begin{array}{c} \hline \\ Transition\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ 3^P_0 \rightarrow {}^3H_4\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ 3^P_0 \rightarrow {}^3H_6\\ 3^P_0 \rightarrow {}^3F_2\\ {}^1D_2 \rightarrow {}^3F_3\\ \end{array}$ |
| Label a Label a b c d e f g | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 520.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 21026 20186 19216 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $^{3}P_{2} \leftarrow ^{3}H_{4}$ $^{3}P_{1} \leftarrow ^{3}H_{4}$ $^{3}P_{0} \leftarrow ^{3}H_{4}$ not assignable | (6) | Label c Label h i j k l m n o p q | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 644.4 682.8 714 725 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 16526 15518 14646 14006 13793 | $\begin{array}{c} Transition\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \end{array}$ $\begin{array}{c} \hline \\ Transition\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ 3^P_0 \rightarrow ^3H_4\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ ^3P_0 \rightarrow ^3H_6\\ ^3P_0 \rightarrow ^3F_2\\ ^1D_2 \rightarrow ^3H_5\\ ^3P_0 \rightarrow ^3F_3\\ ^3P_0 \rightarrow ^3F_3 \end{array}$ |
| Label a Label a b c d e f g | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 520.4 | Energy (cm ⁻¹) 36036 32680 Excitation 28458 24178 22941 22104 21026 20186 19216 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $3P_2 \leftarrow ^3H_4$ $^3P_1 \leftarrow ^3H_4$ $^3P_0 \leftarrow ^3H_4$ not assignable | (6) | Label c Label h i j k l m n o p q | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 644.4 682.8 714 725 | Energy (cm ⁻¹) 23245 Emission 22129 21561 20991 20421 19015 16526 15518 14646 14006 13793 | $\begin{array}{c} Transition\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \end{array}$ $\begin{array}{c} Transition\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ 3P_0 \rightarrow 3H_4\\ \pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n\\ 3P_0 \rightarrow 3H_6\\ 3P_0 \rightarrow 3H_6\\ 3P_0 \rightarrow 3F_2\\ 1D_2 \rightarrow 3H_5\\ 3P_0 \rightarrow 3F_3\\ 3P_0 \rightarrow 3F_3\\ \end{array}$ |
| Label a Label a b c d e f g | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 520.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 21026 20186 19216 19216 | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $^{3}P_{2} \leftarrow ^{3}H_{4}$ $^{3}P_{1} \leftarrow ^{3}H_{4}$ $^{3}P_{0} \leftarrow ^{3}H_{4}$ not assignable | (6) | Label c Label h i j k l m n o p q | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 644.4 682.8 714 725 | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 16526 15518 14646 14006 13793 | $\frac{\text{Transition}}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ $\frac{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $^{3}P_{0} \rightarrow^{3}H_{4}$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $^{3}P_{0} \rightarrow^{3}H_{5}$ $^{3}P_{0} \rightarrow^{3}F_{2}$ $^{1}D_{2} \rightarrow^{3}F_{3}$ $^{3}P_{0} \rightarrow^{3}F_{3}$ |
| Label a b Label a b c d d e f g | λ (nm) 277.5 306 λ (nm) 351.4 413.6 435.9 452.4 475.6 495.4 520.4 520.4 | Energy (cm ⁻¹) 36036 32680 Excitation Energy (cm ⁻¹) 28458 24178 22941 22104 22104 21026 20186 19216 19216 Excitation Excitation | Transition $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ $3P_2 \leftarrow ^3H_4$ $^3P_1 \leftarrow ^3H_4$ $^3P_0 \leftarrow ^3H_4$ not assignableTransition | (6) | Label c Label h i j k l m n o p q q Label | λ (nm) 430.2 λ (nm) 451.9 463.8 476.4 489.7 525.9 605.1 644.4 682.8 714 725 λ (nm) | Energy (cm ⁻¹) 23245 Emission Energy (cm ⁻¹) 22129 21561 20991 20421 19015 16526 15518 14646 14006 13793 Emission Energy (cm ⁻¹) | $\frac{\text{Transition}}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ $\frac{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ $\frac{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ $\frac{3P_0 \rightarrow ^3H_4}{\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n}$ $\frac{3P_0 \rightarrow ^3H_6}{3P_0 \rightarrow ^3F_2}$ $\frac{1D_2 \rightarrow ^3H_5}{3P_0 \rightarrow ^3F_3}$ $\frac{3P_0 \rightarrow ^3F_3}{3P_0 \rightarrow ^3F_3}$ |

| b | 345.9 | 28910 | $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | | d | 416 | 24038 | $^{2}P_{3/2} \rightarrow ^{4}I_{9/2}$ |
|---------------------------------|--|---|--|-----|--------------------------------------|--|---|---|
| | | | | | e | 434.5 | 23015 | ${}^{2}P_{3/2} \rightarrow {}^{4}I_{11/2}$ |
| | | | | | f | 447 | 22371 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | g | 463.7 | 21566 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | h | 479.3 | 20864 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | i | 488.9 | 20454 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | j | 512.9 | 19497 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| | | | | | k | 551.2 | 18142 | ${}^{2}G_{7/2} + {}^{4}G_{5/2} \rightarrow {}^{4}I_{9/2}$ |
| | | | | | 1 | 588.9 | 16981 | ${}^{2}G_{7/2} + {}^{4}G_{5/2} \rightarrow {}^{4}I_{9/2}$ |
| | | | | (8) | | | | |
| | | Excitation | | | | | | |
| Label | λ (nm) | Energy (cm ⁻¹) | Transition | | Label | λ (nm) | Energy (cm ⁻¹) | Transition |
| а | 330.9 | 30221 | $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | | i | 136.2 | 22025 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| u | 550.7 | 50221 | | | 1 | 430.2 | 22925 | <i>n n</i> 01 <i>n n</i> |
| b | 382.6 | 26137 | $\pi \rightarrow \pi^*$ or $n \rightarrow \pi^*$ | | j | 447.3 | 22325 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b c | 382.6 436.9 | 26137 22889 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ ${}^4G_{9/2} \leftarrow {}^6H_{5/2}$ | | j k | 447.3 465.4 | 22925 22356 21487 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b c d | 382.6 436.9 450.4 | 26137 22889 22202 | $\pi \rightarrow \pi^* \text{ or } n \rightarrow \pi^*$ ${}^{4}G_{9/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}M_{17/2}, {}^{4}F_{5/2} \leftarrow {}^{6}H_{5/2}$ | | j k l | 447.3 465.4 486.4 | 22325 22356 21487 20559 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b c d e | 382.6 436.9 450.4 467.4 | 26137 22889 22202 21395 | $\pi \rightarrow \pi^{*} \text{ or } n \rightarrow \pi^{*}$ ${}^{4}G_{9/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}M_{17/2}, {}^{4}F_{5/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{13/2} \leftarrow {}^{6}H_{5/2}$ | | j k l m | 447.3 465.4 486.4 532.7 | 22323 22356 21487 20559 18772 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b c d e f | 382.6 436.9 450.4 467.4 484.6 | 26137 22889 22202 21395 20636 | $\pi \rightarrow \pi^{*} \text{ or } n \rightarrow \pi^{*}$ ${}^{4}G_{9/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}M_{17/2}, {}^{4}F_{5/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{13/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{11/2}, {}^{4}M_{15/2} \leftarrow {}^{6}H_{5/2}$ | | j k l m n | 447.3 465.4 486.4 532.7 558 | 22356 21487 20559 18772 17921 | $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ $\pi^* \rightarrow \pi \text{ or } \pi^* \rightarrow n$ |
| b c d e f g | 382.6 436.9 450.4 467.4 484.6 496.9 | 26137 22889 22202 21395 20636 20125 | $\begin{array}{c} \pi \rightarrow \pi^{*} \text{ or } n \rightarrow \pi^{*} \\ {}^{4}G_{9/2} \leftarrow {}^{6}H_{5/2} \\ {}^{4}M_{17/2}, {}^{4}F_{5/2} \leftarrow {}^{6}H_{5/2} \\ {}^{4}I_{13/2} \leftarrow {}^{6}H_{5/2} \\ {}^{4}I_{11/2}, {}^{4}M_{15/2} \leftarrow {}^{6}H_{5/2} \\ {}^{4}I_{9/2}, {}^{4}G_{7/2} \leftarrow {}^{6}H_{5/2} \end{array}$ | | j k l m n o | 447.3 465.4 486.4 532.7 558 594.9 | 22356 21487 20559 18772 17921 16810 | $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $^{4}G_{5/2} \rightarrow^{6}H_{5/2}$ $^{4}G_{5/2} \rightarrow^{6}H_{7/3}$ |
| b c d e f g h | 382.6 436.9 450.4 467.4 484.6 496.9 511.6 | 26137 22889 22202 21395 20636 20125 19547 | $\pi \rightarrow \pi^{*} \text{ or } n \rightarrow \pi^{*}$ ${}^{4}G_{9/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}M_{17/2}, {}^{4}F_{5/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{13/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{11/2}, {}^{4}M_{15/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{9/2}, {}^{4}G_{7/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{11/2}, \leftarrow {}^{6}H_{5/2}$ | | j k l m n o p | 447.3 465.4 486.4 532.7 558 594.9 639.7 | 22356 21487 20559 18772 17921 16810 15632 | $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $^{4}G_{5/2} \rightarrow^{6}H_{5/2}$ $^{4}G_{5/2} \rightarrow^{6}H_{9/4}$ |
| b c d e f g h | 382.6 436.9 450.4 467.4 484.6 496.9 511.6 | 26137 22889 22202 21395 20636 20125 19547 | $\pi \rightarrow \pi^{*} \text{ or } n \rightarrow \pi^{*}$ ${}^{4}G_{9/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}M_{17/2}, {}^{4}F_{5/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{13/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{11/2}, {}^{4}M_{15/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{9/2}, {}^{4}G_{7/2} \leftarrow {}^{6}H_{5/2}$ ${}^{4}I_{11/2}, \leftarrow {}^{6}H_{5/2}$ | | j k l m n o p q | 447.3 465.4 486.4 532.7 558 594.9 639.7 685.6 | 22325 22356 21487 20559 18772 17921 16810 15632 14586 | $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $\pi^{*} \rightarrow \pi \text{ or } \pi^{*} \rightarrow n$ $^{4}G_{5/2} \rightarrow ^{6}H_{5/2}$ $^{4}G_{5/2} \rightarrow ^{6}H_{9/4}$ $^{4}G_{5/2} \rightarrow ^{6}H_{11/5}$ |





Figure S6.1. Luminescence decay traces for compounds 1-8. The red line is an exponential fit to the data.

Section S7. CIE coordinates and color emission of 3-OHNDS y (1)-(8) compounds.

| | CIE coordinates | | Color emission | |
|---------|-----------------|------|----------------|--|
| | x y | | | |
| 3-OHNDS | 0.14 | 0.1 | blue | |
| 1 | 0.15 | 0.06 | bluish purple | |
| 2 | 2 0.18 | | greenish blue | |
| 3 | 0.26 0.36 | | bluegreen | |
| 4 | 0.33 | 0.28 | purplish pink | |
| 5 | 0.17 | 0.11 | blue | |
| 6 | 6 0.27 | | bluish green | |
| 7 | 7 0.22 | | bluegreen | |
| 8 | 0.31 | 0.32 | white | |

 Table S2. (x,y) CIE coordinates and color emission of 3-OHNDS y (1)-(8) compounds.

Section S8. Squeeze results.

A disordered solvent molecule was identified in the final stages of refinement for the compounds (1)-(4) and (9). This highly disordered region of the asymmetric unit was treated by application of the of the program Squeeze as implemented in Platon which allows for the mathematical compensation of the electron contribution of disordered solvent contained in the voids to the calculated diffraction intensities. The disordered solvent (water molecules) was treated as a diffuse contribution to the scattering without specific atomic coordinates by PLATON/SQUEEZE as is shown in the Table S3.

Table S3. Squeeze located voids, coordinates, volume and content for compounds (1)-(4) and (9).

| Compound | Coordinates | Volume | Electrons | No. Water |
|----------|----------------------|--------|-----------|-----------|
| | x,y,z | | | molecules |
| (1) | 0.000,0.500, -0.013 | 131 | 26 | 3.25 |
| | 0.000,0.500, -0.013 | 131 | 26 | 3.25 |
| (2) | 0.000, 0.500,-0.015 | 130 | 24 | 3 |
| | 0.500, 0.000, 0.001 | 130 | 24 | 3 |
| (3) | 0.000, 0.500, -0.015 | 130 | 20 | 2.5 |
| | 0.500, 1.000, 0.009 | 130 | 20 | 2.5 |
| (4) | 0.000, 0.500, -0.017 | 149 | 15 | 1.9 |
| | 0.500, 1.000, 0.036 | 149 | 15 | 1.9 |
| (9) | 0.000, 0.000, 0.500 | 120 | 30 | 3.8 |
| | 0.500, 0.500, 0.000 | 120 | 30 | 3.8 |