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Electronic Supplementary Material (ESI) for DALTON TRANSACTIONS

## A Photoluminescent Thermometer made from a Thermoresponsive Tetranuclear Gold Complex and Phosphor N630


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## Contents

Fig. s1. TGA curve of $1 \cdot E t O H$ from room temperature to $500^{\circ} \mathrm{C}$. ................................................................ S2
Fig. s2. IR spectra of compound 1 and $\mathrm{H}_{2} \mathrm{mba}$.
S2
Fig. s3. ${ }^{1} \mathrm{H},{ }^{13} \mathrm{C}$ and ${ }^{31}$ P NMR spectra of 1 in DMSO-d 6 . $\cdot$.......................................................................... 3
Fig. s4. Solid-state excitation (black) and emission (green) spectra of 1-EtOH at room temperature.
Fig. s5. PL intensity of 1 over five cycles between 80 and 300 K and between 300 and 370K......................................S4

Fig. s6. Emission spectra of N630 at 80-300 K (left) and at 300-370 K (right) at an excitation wavelength of 370 nm $\cdots \cdot$. 4

Fig. s7. Solid-state UV-Vis spectra of compound $\mathbf{1}$ at 295, 325 and 355 K• S5

Table s1. Selected crystallographic data and refinement parameters for 1•EtOH at different temperatures. $\cdots \cdots \cdots \cdots$.......S5
Table s2. Selected Bond Lengths and Angels of 1•EtOH at different temperatures. .............................................................


Fig. s1. TGA curve of $1 \cdot \mathrm{EtOH}$ from room temperature to $500^{\circ} \mathrm{C}$.


Fig. s2. IR spectra of compound 1 (upper) and $\mathrm{H}_{2} \mathrm{mba}$ (lower).


Fig. s3. ${ }^{1} \mathrm{H},{ }^{13} \mathrm{C}$ and ${ }^{31} \mathrm{P}$ NMR spectra of 1 in DMSO-d $d_{6}$.


Fig. s4. Solid-state excitation (black) and emission (green) spectra of $1 \cdot \mathrm{EtOH}$ at room temperature.


Fig. s5. PL intensity of 1 over five cycles between 80 and 300 K (left) and between 300 and 370 K (right). The excitation wavelength was 370 nm .


Fig. s6. Emission spectra of N 630 at $80-300 \mathrm{~K}$ (left) and at 300-370 K (right) at an excitation wavelength of 370 nm .


Fig. s7. Solid-state UV-Vis spectra of compound 1 at 295, 325 and 355 K

Table s1. Selected crystallographic data and refinement parameters for $1 \cdot \mathrm{EtOH}$ at different temperatures.

| Temperature | 110 K | 140 K | 180 K | 220 K | 260 K | 300 K |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Empirical formula | C85H77Au4ClN4O7P4S3 |  |  |  |  |  |
| Formula weight | 2309.88 |  |  |  |  |  |
| Crystal system | triclinic |  |  |  |  |  |
| Space group | $P_{1}$ |  |  |  |  |  |
| a/ $\AA$ | 11.2814(9) | 11.2999(9) | 11.3296(10) | 11.3392(6) | 11.3501(6) | 11.3650(7) |
| b/ $\AA$ | 16.5641(14) | 16.5823(13) | 16.6117(14) | 16.6308(9) | 16.6508(9) | 16.6659(9) |
| c/ $\AA$ | 23.6076(19) | 23.6305(19) | 23.632(2) | 23.7027(13) | 23.7568(13) | 23.8298(13) |
| $\alpha{ }^{\circ}$ | 81.379(3) | 81.265(3) | 81.126(4) | 80.931(2) | 80.641(2) | 80.294(2) |
| $\beta{ }^{\circ}$ | 89.680(4) | 89.613(4) | 89.448(4) | 89.323(2) | 89.174(3) | 89.011(2) |
| $\gamma /{ }^{\circ}$ | 73.274(3) | 73.337(3) | 73.432(4) | 73.566(2) | 73.746(2) | 73.898(2) |
| $V / \AA^{3}$ | 4173.8(6) | 4189.5(6) | 4209.3(6) | 4231.1(4) | 4250.6(4) | 4272.3(4) |
| Z | 2 | 2 | 2 | 2 | 2 | 2 |
| $\rho_{\text {cald }} / \mathrm{g} . \mathrm{cm}^{3}$ | 1.838 | 1.831 | 1.822 | 1.813 | 1.805 | 1.796 |
| $\mu / \mathrm{mm}^{-1}$ | 10.307 | 10.269 | 10.221 | 10.168 | 10.121 | 10.070 |
| $F(000)$ | 2224 | 2224 | 2224 | 2224 | 2224 | 2224 |
| $R_{1}{ }^{\text {a }}$ | 0.0324 | 0.0324 | 0.0367 | 0.0383 | 0.0442 | 0.0594 |
| $w R_{2}{ }^{\text {b }}$ | 0.0825 | 0.0818 | 0.0926 | 0.1027 | 0.1273 | 0.1932 |
| GOF ${ }^{\text {c }}$ | 1.057 | 1.040 | 1.046 | 1.057 | 1.065 | 1.085 |

${ }^{\mathrm{a}} R_{1}=\Sigma| | F_{o}\left|-\left|F_{c} \| / \Sigma\right| F_{o}\right|,{ }^{\mathrm{b}} \mathrm{wR}_{2}=\left\{\Sigma \mathrm{w}\left(F_{o}{ }^{2}-F_{c}{ }^{2}\right)^{2} / \Sigma \mathrm{w}\left(F_{o}{ }^{2}\right)^{2}\right\}^{1 / 2}$. ${ }^{\mathrm{c}} \mathrm{GOF}=\left\{\Sigma \mathrm{w}\left(\left(F_{o}{ }^{2}-F_{c}{ }^{2}\right)^{2}\right) /(n-p)\right\}^{1 / 2}$, where $n=$ number of reflection and $p=$ total number of parameters refined.

Table s2. Selected Bond Lengths $(\AA)$ and Angels $\left({ }^{\circ}\right)$ of $\mathbf{1} \cdot \mathrm{EtOH}$ at different temperatures.

| Temperature | $\mathbf{1 1 0} \mathbf{K}$ | $\mathbf{1 4 0} \mathbf{K}$ | $\mathbf{1 8 0} \mathbf{K}$ | $\mathbf{2 2 0} \mathbf{K}$ | $\mathbf{2 6 0} \mathbf{K}$ | $\mathbf{3 0 0} \mathbf{K}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Au2-Au3 | $3.0710(4)$ | $3.0788(3)$ | $3.0862(4)$ | $3.0987(4)$ | $3.1106(5)$ | $3.1287(7)$ |
| Au2-C11 | $2.2994(11)$ | $2.2982(12)$ | $2.2965(13)$ | $2.2974(14)$ | $2.2943(17)$ | $2.292(2)$ |
| Au1-P1 | $2.2602(11)$ | $2.2589(12)$ | $2.2567(14)$ | $2.2581(14)$ | $2.2580(17)$ | $2.261(3)$ |
| Au2-P2 | $2.2320(11)$ | $2.2313(11)$ | $2.2329(13)$ | $2.2335(13)$ | $2.2324(16)$ | $2.235(2)$ |
| Au3-P3 | $2.2607(12)$ | $2.2592(13)$ | $2.2587(15)$ | $2.2573(16)$ | $2.255(2)$ | $2.252(3)$ |
| Au4-P4 | $2.2547(13)$ | $2.2553(13)$ | $2.2513(15)$ | $2.2519(16)$ | $2.251(2)$ | $2.251(3)$ |
| Au1-S1 | $2.3102(11)$ | $2.3097(12)$ | $2.3092(13)$ | $2.3092(14)$ | $2.3089(17)$ | $2.304(3)$ |
| Au3-S2 | $2.3119(13)$ | $2.3109(14)$ | $2.3091(17)$ | $2.3061(19)$ | $2.308(2)$ | $2.309(4)$ |
| Au4-S3 | $2.2952(12)$ | $2.2953(13)$ | $2.2933(15)$ | $2.2893(17)$ | $2.290(2)$ | $2.290(3)$ |
| P1-Au1-S1 | $174.35(4)$ | $174.43(4)$ | $174.49(5)$ | $174.53(5)$ | $174.64(6)$ | $174.77(9)$ |
| P2-Au2-Cl1 | $177.44(4)$ | $177.35(4)$ | $177.19(5)$ | $177.05(5)$ | $177.01(6)$ | $176.82(9)$ |
| P2-Au2-Au3 | $98.12(3)$ | $98.27(3)$ | $98.42(3)$ | $98.85(4)$ | $99.22(4)$ | $99.70(6)$ |
| C11-Au2-Au3 | $84.37(3)$ | $84.33(3)$ | $84.35(4)$ | $84.08(4)$ | $83.76(5)$ | $83.48(7)$ |
| P3-Au3-S2 | $174.68(5)$ | $174.73(5)$ | $174.81(6)$ | $174.98(7)$ | $175.03(8)$ | $174.90(13)$ |
| P3-Au3-Au2 | $102.28(3)$ | $102.40(3)$ | $102.30(4)$ | $102.45(4)$ | $102.63(5)$ | $102.80(7)$ |
| S2-Au3-Au2 | $82.92(4)$ | $82.77(4)$ | $82.77(5)$ | $82.50(5)$ | $82.28(7)$ | $82.22(10)$ |
| P4-Au4-S3 | $174.25(4)$ | $174.40(5)$ | $174.56(6)$ | $174.72(6)$ | $174.99(8)$ | $175.34(11)$ |

