**Supplementary Information**

Synthesis, characterization and structural determination of copper(II) complexes with alkyl derivatives of hydroxybenzophenones

CRISTIANE BATISTA GONÇALVES, MARIA VANDA MARINHO, DANIELLE FERREIRA DIAS, MARCELO HENRIQUE DOS SANTOS, FELIPE TERRA MARTINS and ANTÔNIO CARLOS DORIGUETTO\*

**S1 - IR spectra**



Figure S1. Infrared spectra of LFQM-115 and **1**.



Figure S2. Infrared spectra of LFQM-116 and **2**.



Figure S3. Infrared spectra of LFQM-117 and **3**.



Figure S4. Infrared spectra of octyloxy and **4**.

**S2 - Powder X-ray diffraction data**



Figure S5. Experimental (LFQM-115 - Exp.) and calculated (LFQM-115 - Calc.) PXRD patterns of LFQM-115.



Figure S6. Experimental (LFQM-116 - Exp.) and calculated (LFQM-116 - Calc.) PXRD patterns of LFQM-116.



Figure S7. Experimental (LFQM-117 - Exp.) and calculated (LFQM-117 - Calc.) PXRD patterns of LFQM-117.



Figure S8. Experimental (octyloxy - Exp.) and calculated (octyloxy - Calc.) PXRD patterns of octyloxy.



Figure S9. Experimental (**1** - Exp.) and calculated (**1** - Calc.) PXRD patterns of **1**. Spurious peaks indicated by arrows.



Figure S10. Experimental (**2** - Exp.) and calculated (**2** - Calc.) PXRD patterns of **2**. Spurious peaks indicated by arrows.



Figure S11. Experimental (**3** – Exp.) and calculated (**3** – Calc.) PXRD patterns of **3**. Spurious peaks indicated by arrows.



(a)



(b)

Figure S12. (a)Experimental (**4** – Exp.) and simulated (**4** – Calc.) PXRD patterns of **4**. (b) The same patterns with zoom in order to highlight the peaks with low relative intensity.

**S3 - Thermogravimetry and differential thermal analysis curves**



Figure S13. TGA / DTA curves of LFQM-116 and LFQM-117.



(a)



(b)

Figure S14. TG (a) / DTA (b) curves of **1**-**4**.

**S4 – Single crystal X-ray diffraction extra results**

Table S1. Hydrogen bonds for LFQM-116 (Å and °), where *d = distance;* <(D-H-A) *= angle;* D = donor and A = acceptor.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | | d(D-H) | | d(H…A) | | d(D…A) | <(D-H-A) |
| O1-H1...O2 | | *0.93(2)* | | *0.93(2)* | | *0.93(2)* | *0.93(2)* |
| O1’-H1’...O2’ | | *1.73(3)* | | *1.73(3)* | | *1.73(3)* | *1.73(3)* |
| C6-H6...O2' | | *2.560(2)* | | *2.560(2)* | | *2.560(2)* | *2.560(2)* |
| C3’- H3’...O2(i) | | *147(2)* | | *147(2)* | | *147(2)* | *147(2)* |
| C10- H10…O1(ii) | | *0.97(3)* | | *0.97(3)* | | *0.97(3)* | *0.97(3)* |
| C10’- H10’…O1’(iii) | | *1.65(3)* | | *1.65(3)* | | *1.65(3)* | *1.65(3)* |
|  |  | |  | |  | | |

*Symmetry codes: (i) -x-1, -y+1, -z; (ii) -x, -y+2, -z+1; (iii) -x, -y+1, ‑z+1.*



Figure S15. Centrosymmetric dimer of the LFQM-116 molecules A and B linked together to form a chain growing along [212]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Figure S16. A section projected onto (101) of the supramolecular two-dimensional assembly of LFQM-116. The chain propagation along [010] is evident. Hydrogen bonds are shown as dashed lines. Displacement ellipsoids are drawn at 25% probability level for clarity. The aromatic rings in margent highlight molecules having the conformer B of the asymmetric unit. Symmetry codes in (a): (i) –x-1, -y+1, -z.



Figure S17. View of LFQM-116 showing its partial packing onto plane *ac*. The color scheme represents the conformer A (blue) and B (green).



Figure S18. Least-square planes calculated through carbons of the substituted (in green) and unsubstituted (in yellow) aromatic rings and prenyl (margent) moiety of LFQM-117. The angles between the calculated least-square planes are shown.



Figure S19. Overlay of the benzophenonic backbone of the LFQM-115 (CCDC HMXBZP) [54], octyloxy (CCDC KOSZIB) [55], 2,4-dihydroxybenzophenone (CCDC DHXBZP) [56], LFQM-116 and LFQM-117). The structures were matched considering the circled atoms. The object in orange represents the least-square plane calculated through carbons of the substituted aromatic ring of each compared molecule. The angles between the calculated least-square planes through the substituted and unsubstituted aromatic rings of each compared molecule are given. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Figure S20. View of LFQM-117 showing its partial packing onto plane *ac*. The color scheme represents the symmetry operations of *Pbca* space group plus translations. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Figure S21. View of LFQM-115 (CCDC HMXBZP) [54] showing its partial packing onto plane *ac*. The color scheme represents the symmetry operations of Pbca space group plus translations. The unit cell parameter change, occurring mainly along the unit cell *c* axis (26.37(2) for LFQM-117 *vs.* 32.865(1) Å for LFQM-115), is a direct consequence of the volume difference of the substituent at the 4-position (prenyl *vs.* metoxyl) (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Figure S22. View of the stacked complex units that is the common supramolecular synthon of the [Cu(bpo)2], **1**, **2**, **3** and **4** structures. The molecular stacking occurs along the *a* unit cell axis for [Cu(bpo)2] and along the *b* unit cell axis for the complexes reported here. The CuII cations are in green and the hydrogens were omitted for clarity. The dotted line represents the shortest Cu…Cu distances (SD) whose values are also included. [Cu(bpo)2] view was generated from the CCDC UHUDIM [57]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)