Supporting Information

Schiff bases functionalized with t-butyl groups as adequate ligands to extended assembly of Cu(II) helicates

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1. Schiff base ligands H2L1 and H2L2



Figure S1. 1H NMR spectra of H2L1 (400 MHz, acetone-d6, r.t., δ (m, nH, Hx, J)): 12.98 (s, 2H, H1), 8.92 (s, 2H, H2), 7.91 (d, J= 2.5 Hz, 2H, H3); 7.47 (dd, J= 8.7, 2.5 Hz, 2H, H4), 7.37 (s, 8H, H5+H6); 6.89 (d, J= 8.7 Hz, 2H, H7); 4.08 (s, 2H, H8), 1.32 (s, 18H, H9).



Figure S2. 1H NMR spectra of H2L2 (400 MHz, acetone-d6, r.t., δ (m, nH, Hx, J)): 14.01 (s, 2H, H1), 8.90 (s, 2H, H2), 7.44-7.37 (m, 12H, H3-H6); 6.89 (t, J= 7 Hz, 2H, H7); 4.09 (s, 2H, H8), 1.44 (s, 18H, H9).

1. Copper(II) helicates derived from Schiff base ligands



Figure S3. Infrared spectra superposition of H2L1 (pink) and [Cu2(L1)2] (blue).



Figure S4. Intermolecular CH···π interactions in the crystal lattice of the [Cu2(L1)2]·4CH3CN helicate.



Figure S5. Intermolecular π ···π interactions in the crystal lattice of the [Cu2(L2)2]·CH3CN helicate.

Table S1. Main crystallographic data for helicates [Cu2(L1)2]·4CH3CN and [Cu2(L2)2]·CH3CN.

|  |  |  |
| --- | --- | --- |
|  | [Cu2(L1)2]·4CH3CN | [Cu2(L2)2]·CH3CN |
| Molecular formula | C72H75N5O4Cu2 | C72H75N5O4Cu2 |
| Molecular weight | 1329.11 | 1201.45 |
| Spatial group | *I2/a* | *P* |
| Crystalline system | Monoclinic | Triclinic |
| Crystal size/mm | 0.20 × 0.19 × 0.07 | 0.05 × 0.04 × 0.02 |
| a/Å | 18.7980(5) | 11.4703(5) |
| b/Å | 17.0029(5) | 13.3929(5) |
| c/Å | 23.3318(9) | 20.4608(7) |
| /º | 90 | 95.462(3) |
| /º | 109.65 (10) | 101.556(3) |
| /º | 90 | 100.206(3) |
| Temperature/K | 100 | 100 |
| Volume/Å3 | 7023.0 (4) | 2667.0(2) |
| Z | 4 | 2 |
| Measured reflexions | 45292 | 41389 |
| Unique reflexions [Rint] | 7172 [0.044] | 10230 [0.159] |
| /mm1 | 0.661 | 1.300 |
| Residues/e Å3 | 2.11 and -0.53 | 0.35 and -0.79 |
| R | 0.065 | 0.068 |
| *w*R | 0.109 | 0.187 |

Table S2. Main bond distances and angles for [Cu2(L1)2]·4CH3CN helicate.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond distances (Å) | | | | | |
| N1—Cu1 | 1.967 (2) | O1—Cu1 | 1.8935 (18) | N1—Cu1 | 1.967 (2) |
| N2—Cu1i | 1.962 (2) | O2—Cu1i | 1.8907(17) | N2—Cu1i | 1.962 (2) |
| Bond angles (⁰) | | | | | |
| O1—Cu1—O2i | 92.07(8) | O2—Cu1i—N1i | 142.00(9) | O1—Cu1—O2i | 92.07(8) |
| O2i—Cu1—N2i | 94.90(8) | O1i—Cu1i—N1i | 94.89(8) | O2i—Cu1—N2i | 94.90(8) |
| O1—Cu1—N2i | 144.84(9) | N2—Cu1i—N1i | 100.41(8) | O1—Cu1—N2i | 144.84(9) |

Table S3. Main bond distances and angles for [Cu2(L2)2]·CH3CN helicate.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Bond distances (Å) | | | | | |
| N1—Cu1 | 1.963 (5) | O1—Cu1 | 1.885 (4) | N1—Cu1 | 1.963 (5) |
| N2—Cu2 | 1.943 (4) | O2—Cu2 | 1.903 (4) | N2—Cu2 | 1.943 (4) |
| N3—Cu2 | 1.973 (5) | O3—Cu2 | 1.875 (4) | N3—Cu2 | 1.973 (5) |
| N4—Cu1 | 1.942 (5) | O4—Cu1 | 1.895 (3) | N4—Cu1 | 1.942 (5) |
| Bond angles (⁰) | | | | | |
| O4—Cu1—O1 | 95.32 (16) | O2—Cu2—O3 | 92.28 (16) | O4—Cu1—O1 | 95.32 (16) |
| O4—Cu1—N1 | 139.98 (18) | O2—Cu2—N3 | 147.87 (18) | O4—Cu1—N1 | 139.98 (18) |
| O1—Cu1—N1 | 93.02 (18) | O3—Cu2—N3 | 94.45 (18) | O1—Cu1—N1 | 93.02 (18) |
| O4—Cu1—N4 | 94.07 (17) | O2—Cu2—N2 | 92.71 (18) | O4—Cu1—N4 | 94.07 (17) |
| O1—Cu1—N4 | 146.43 (19) | O3—Cu2—N2 | 150.31 (19) | O1—Cu1—N4 | 146.43 (19) |
| N1—Cu1—N4 | 100.18 (19) | N3—Cu2—N2 | 96.72 (19) | N1—Cu1—N4 | 100.18 (19) |
| O4—Cu1—O1 | 95.32 (16) | O2—Cu2—O3 | 92.28 (16) | O4—Cu1—O1 | 95.32 (16) |
| O4—Cu1—O1 | 95.32 (16) | O2—Cu2—O3 | 92.28 (16) | O4—Cu1—O1 | 95.32 (16) |