Supplementary material

**Table 2** Selected bond lengths/Å and angles/° for the compounds

|  |  |  |  |
| --- | --- | --- | --- |
| HL2 |  |  |  |
| C6-N2 | 1.272(3) | N2-N3 | 1.375(2) |
| N3-C7 | 1.356(3) | C7-O1 | 1.229(3) |
| C20-N5 | 1.273(3) | N5-N6 | 1.369(2) |
| N6-C21 | 1.360(3) | C21-O3 | 1.229(2) |
| C6-N2-N3 | 116.4(2) | N2-N3-C7 | 118.6(2) |
| C20-N5-N6 | 116.9(2) | N5-N6-C21 | 118.1(2) |
| **1** |  |  |  |
| Cu1-N1 | 2.007(3) | Cu1-N2 | 1.928(3) |
| Cu1-O1 | 1.965(3) | Cu1-O2 | 2.284(4) |
| Cu1-N4 | 1.927(4) |  |  |
| C6-N2 | 1.280(4) | N2-N3 | 1.375(4) |
| N3-C7 | 1.333(4) | C7-O1 | 1.277(5) |
| N4-Cu1-N2 | 159.33(18) | N4-Cu1-O1 | 99.50(14) |
| N2-Cu1-O1 | 79.18(12) | N4-Cu1-N1 | 97.74(15) |
| N2-Cu1-N1 | 80.75(12) | O1-Cu1-N1 | 159.48(13) |
| N4-Cu1-O2 | 111.53(19) | N2-Cu1-O2 | 89.14(13) |
| O1-Cu1-O2 | 90.15(14) | N1-Cu1-O2 | 93.81(15) |
| C6-N2-N3 | 124.4(3) | N2-N3-C7 | 107.2(3) |
| **2** |  |  |  |
| Zn1-N1 | 2.1462(16) | Zn1-N2 | 2.1149(16) |
| Zn1-Cl1 | 2.2233(6) | Zn1-Cl2 | 2.2348(6) |
| Zn1-O1 | 2.2979(14) |  |  |
| N2-Zn1-N1 | 74.91(6) | N2-Zn1-Cl1 | 115.82(5) |
| N1-Zn1-Cl1 | 101.84(5) | N2-Zn1-Cl2 | 124.21(5) |
| N1-Zn1-Cl2 | 103.10(5) | Cl1-Zn1-Cl2 | 118.93(3) |
| N2-Zn1-O1 | 70.54(5) | N1-Zn1-O1 | 145.28(6) |
| Cl1-Zn1-O1 | 96.04(5) | Cl2-Zn1-O1 | 93.65(4) |

**Table 3** Hydrogen bond distances (Å) and bond angles (°) for the compounds

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *D*–H∙∙∙*A* | *d*(*D*–H) | *d*(H∙∙∙*A*) | *d*(*D*∙∙∙*A*) | Angle (*D*–H∙∙∙*A*) |
| HL2 |  |  |  |  |
| O5–H5B∙∙∙N1 | 0.85(1) | 2.18(2) | 2.982(3) | 157(2) |
| O5–H5A∙∙∙O3 | 0.85(1) | 1.99(1) | 2.808(2) | 162(3) |
| O6–H6B∙∙∙O1i | 0.85(1) | 1.99(1) | 2.830(3) | 165(3) |
| O6–H6A∙∙∙N4i | 0.85(1) | 2.19(2) | 2.981(3) | 155(3) |
| N3–H3∙∙∙O6 | 0.86 | 2.04 | 2.863(3) | 161(3) |
| N6–H6C∙∙∙O5ii | 0.86 | 2.07 | 2.898(2) | 162(3) |
| **1** |  |  |  |  |
| O2–H2∙∙∙N3iii | 0.85(1) | 1.99(2) | 2.840(4) | 171(4) |
| **2** |  |  |  |  |
| O3–H3B∙∙∙O1i | 0.82 | 2.26 | 2.997(2) | 149(3) |
| N3–H3∙∙∙O3 | 0.89(1) | 1.93(1) | 2.785(2) | 161(3) |

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



Fig. 1s. IR data for complex 1.



Fig. 2s. UV-Vis data for complex 1 in methanol.



Fig. 3s. IR data for complex 2.



Fig. 4s. UV-Vis data for complex 2 in methanol.



Fig. 5s. UV-Vis spectrum of complex 1 in aqueous media.



Fig. 6s. UV-Vis spectrum of complex 2 in aqueous media.