

Electronic Supplementary Information

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Efficient preparation of multimetallic ONO-based Schiff base complexes of nickel(II) and copper(II)

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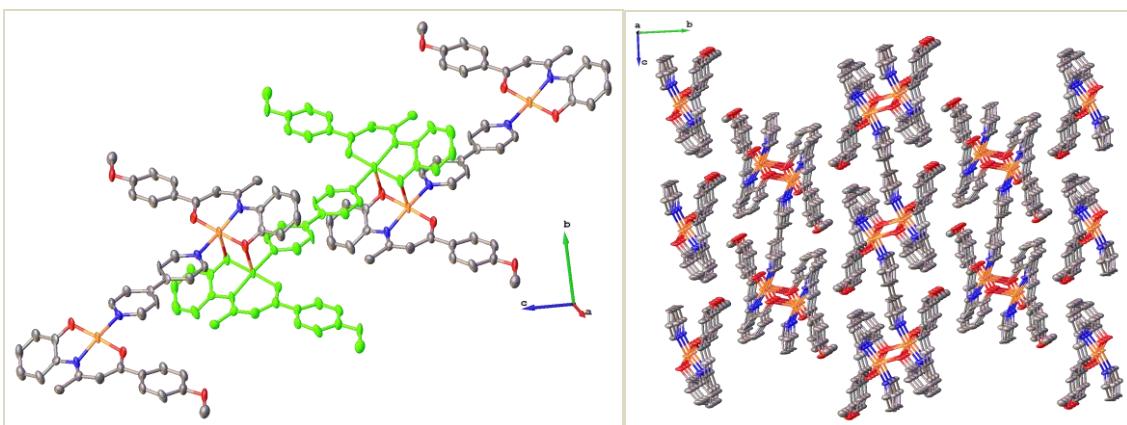


Fig. S1 Growing packing perspective of complex **3** (top), forming a coordination polymer in the crystal lattice (complex unit in green). Packing view of **3** (bottom) showing a perspective through the “a” axis. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are drawn at 70% probability.

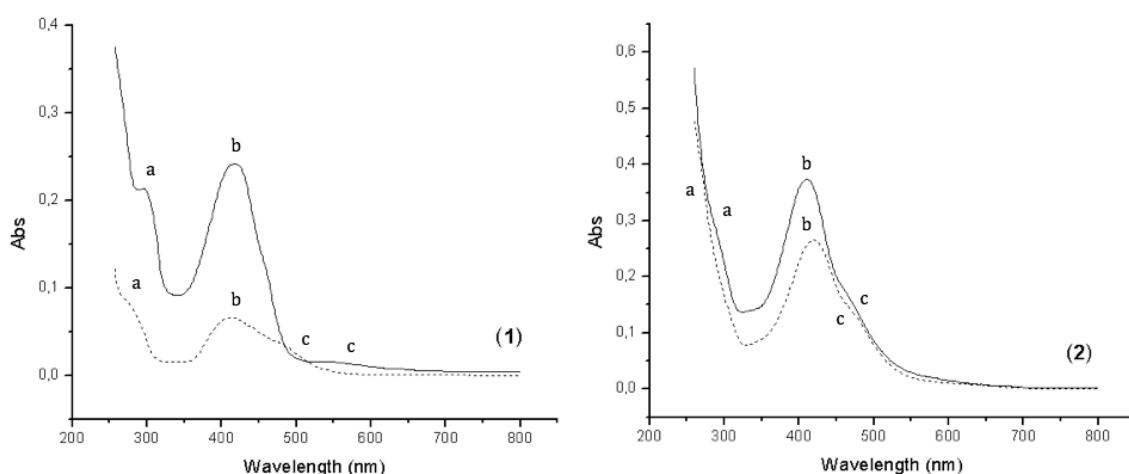


Fig. S2 Experimental electronic spectra registered at 298 K in CH_2Cl_2 (full line) and DMSO (dashed line) of (**1**) (left) and (**2**) (right).

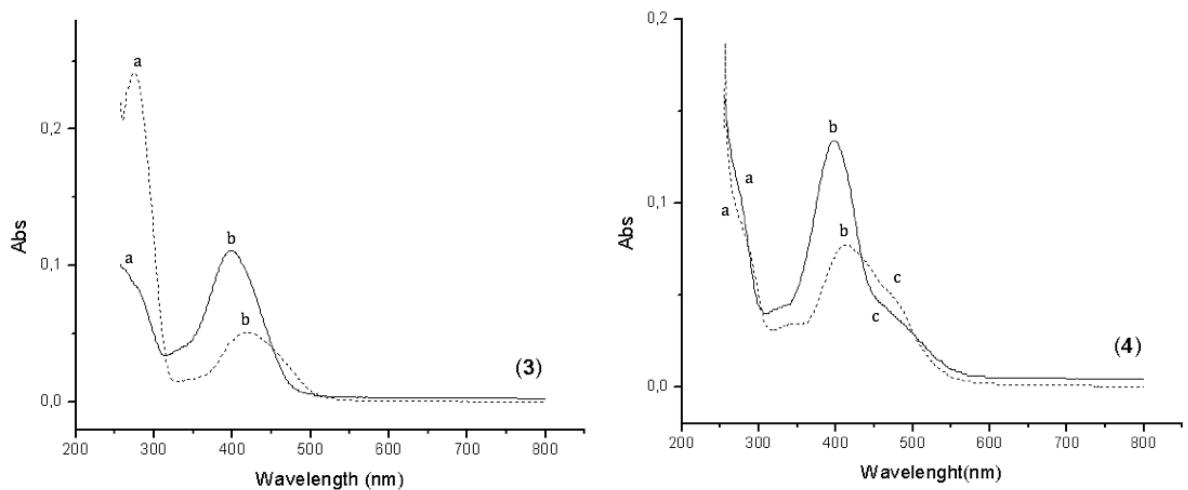


Fig. S3 Experimental electronic spectra registered at 298 K in CH_2Cl_2 (full line) and DMSO (dashed line) of (**3**) (left) and (**4**) (right).

Table S1. Selected bond distances (\AA) and angles ($^\circ$) for compounds **1** and **3**

| | 1 | 3 |
|-----------------|------------------------|-------------------------|
| Bond distances | | |
| O(1)-C(1) | 1.340(5) | 1.342(8) |
| C(1)-C(2) | 1.395(6) | 1.416(9) |
| N(1)-C(2) | 1.432(5) | 1.428(8) |
| N(1)-C(7) | 1.337(5) | 1.328(8) |
| C(7)-C(9) | 1.406(5) | 1.404(8) |
| C(9)-C(10) | 1.369(4) | 1.401(9) |
| C(10)-O(2) | 1.312(5) | 1.307(8) |
| N(2)-C(18) | 1.311(5) | 1.369(7) |
| N(2)-C(22) | 1.328(5) | 1.342(8) |
| C(20)-C(20') | 1.482(8) ^{#1} | 1.500(12) ^{#2} |
| Bond angles | | |
| M(1)-O(1)-C(1) | 113.8(3) | 110.4(4) |
| M(1)-N(1)-C(2) | 110.7(3) | 110.8(4) |
| M(1)-N(1)-C(7) | 123.2(3) | 123.1(4) |
| M(1)-O(2)-C(10) | 125.4(3) | 123.0(4) |
| N(1)-C(7)-C(9) | 122.3(4) | 120.6(6) |
| C(7)-C(9)-C(10) | 127.7(4) | 128.0(7) |
| C(9)-C(10)-O(2) | 123.6(4) | 124.1(6) |

$\text{M} = \text{Ni}$, **1**; Cu , **3**. Symmetry transformations used to generate equivalent atoms: #1 $-\text{x}+1, -\text{y}+2, -\text{z}$; #2 $-\text{x}+2, -\text{y}, -\text{z}+1$

Table S2. Selected bond distances (\AA) and angles ($^\circ$) for compound **2**

| Bond distances | | | |
|------------------|----------|-------------------|----------|
| O(1)-C(1) | 1.330(4) | O(3)-C(31) | 1.337(5) |
| C(1)-C(2) | 1.404(5) | C(31)-C(32) | 1.409(6) |
| N(1)-C(2) | 1.432(4) | N(3)-C(32) | 1.413(5) |
| N(1)-C(7) | 1.331(5) | N(3)-C(37) | 1.337(5) |
| C(7)-C(9) | 1.401(5) | C(37)-C(39) | 1.414(5) |
| C(9)-C(10) | 1.378(5) | C(39)-C(40) | 1.373(5) |
| C(10)-O(2) | 1.307(4) | C(40)-O(4) | 1.304(4) |
| N(2)-C(21) | 1.335(4) | N(4)-C(51) | 1.359(4) |
| N(2)-C(25) | 1.351(5) | N(4)-C(55) | 1.342(5) |
| C(23)-C(53) | 1.488(5) | | |
| Fe(1)-C(Cp) | 2.034(4) | Fe(2)-C(Cp) | 2.043(4) |
| Fe(1)-C(Cp') | 2.037(4) | Fe(2)-C(Cp') | 2.041(4) |
| Bond angles | | | |
| Ni(1)-O(1)-C(1) | 112.2(2) | Ni(2)-O(31)-C(32) | 112.0(3) |
| Ni(1)-N(1)-C(2) | 110.1(2) | Ni(2)-N(3)-C(32) | 110.5(3) |
| Ni(1)-N(1)-C(7) | 110.1(2) | Ni(2)-N(3)-C(37) | 124.6(3) |
| Ni(1)-O(2)-C(10) | 124.6(2) | Ni(2)-O(4)-C(40) | 125.1(2) |
| N(1)-C(7)-C(9) | 121.9(4) | N(3)-C(37)-C(39) | 121.2(4) |
| C(7)-C(9)-C(10) | 125.8(4) | C(37)-C(39)-C(40) | 125.3(4) |
| C(9)-C(10)-O(2) | 124.2(4) | C(39)-C(40)-O(4) | 124.4(3) |

Abbreviations : Cp = C_5H_5 , Cp' = C_5H_4

TableS3. Selected bond distances (\AA) and angles ($^\circ$) for compound **5**

| 5A | 5B | | |
|--------------------------------|------------|--------------------------------|------------|
| Bond distances | | | |
| O(1)-C(1) | 1.349(3) | O(3)-C(21) | 1.341(3) |
| C(1)-C(2) | 1.416(3) | C(21)-C(22) | 1.409(3) |
| N(1)-C(2) | 1.420(3) | N(2)-C(22) | 1.423(3) |
| N(1)-C(7) | 1.325(3) | N(2)-C(27) | 1.327(3) |
| C(7)-C(9) | 1.409(3) | C(27)-C(29) | 1.419(3) |
| C(9)-C(10) | 1.384(3) | C(29)-C(30) | 1.390(3) |
| C(10)-O(2) | 1.296(3) | C(30)-O(4) | 1.295(3) |
| Cu(1)-Cu(1) ^{#1} | 3.0369(6) | Cu(2)-Cu(2) ^{#2} | 3.0096(6) |
| Fe(1)-C(Cp) | 2.050(3) | Fe(2)-C(Cp) | 2.042(3) |
| Fe(1)-C(Cp') | 2.047(3) | Fe(2)-C(Cp') | 2.038(2) |
| Bond angles | | | |
| Cu(1)-O(1)-Cu(1) ^{#1} | 103.20(7) | Cu(2)-O(3)-Cu(2) ^{#2} | 102.43(7) |
| O(1)-Cu(1)-O(1) ^{#1} | 76.90(7) | O(3)-Cu(2)-O(3) ^{#2} | 77.57(7) |
| Cu(1)-O(1)-C(1) | 112.57(14) | Cu(2)-O(3)-C(21) | 113.19(14) |
| Cu(1)-N(1)-C(2) | 110.82(14) | Cu(2)-N(2)-C(22) | 111.26(14) |
| Cu(1)-N(1)-C(7) | 121.10(16) | Cu(2)-N(2)-C(27) | 120.53(15) |
| Cu(1)-O(2)-C(10) | 121.70(14) | Cu(2)-O(4)-C(30) | 122.14(14) |
| N(1)-C(7)-C(9) | 122.1(2) | N(2)-C(27)-C(29) | 121.8(2) |
| C(7)-C(9)-C(10) | 128.4(2) | C(27)-C(29)-C(30) | 127.3(2) |
| C(9)-C(10)-O(2) | 125.7(2) | C(29)-C(30)-O(4) | 125.6(2) |

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1 #2 -x+2,-y,-z+2. Abbreviations : Cp = C_5H_5 , Cp' = C_5H_4

Table S4. Metrical parameters of the ferrocenyl units in compounds **2** and **5**

| Compd | Fe-Cp _{CNT} (Å) | Fe-Cp' _{CNT} (Å) | Cp _{CNT} -Fe-Cp' _{CNT} (°) | Cp/Cp' (°) |
|-----------|--------------------------|---------------------------|--|----------------|
| 2 | 1.652, 1.639 | 1.643, 1.639 | 178.72, 178.62 | 1.0(3), 1.7(2) |
| 5A | 1.658 | 1.652 | 179.41 | 4.4(2) |
| 5B | 1.640 | 1.648 | 179.53 | 3.5(2) |

Abbreviations: Cp = C₅H₅, Cp' = C₅H₄, CNT = centroid.