**Supporting Information**

Incorporating ferrocenecarboxylato(-1) into a [CuI2(μ-dppm)2]2+ (dppm = bis(diphenylphosphino)methane) scaffold for hydrogen peroxide sensing

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**Characterization**

**Figures：**



1. The IR spectrum of complex **1**.



1. The UV-visible spectrum of **1** in CH3OH. (**ε**max441 nm = 321.9 L·mol-1·cm-1)



1. Solution 1H NMR (CD2Cl2) spectrum of complex **1**. δ(ppm) 1.9 (6H, s, C*H*3CN), 3.40 (4H, d, C*H*2), 4.4 (5H, s, ղ5-C5*H*5), 4.5 (2H, s, ղ5-C(C*H*)2(CH)2COO-), 5.0 (2H, s, ղ5-C(CH)2(C*H*)2COO-), 7.1, 7.2, 7.3, 7.4 (40 H, s, br, *Ph*).



1. 31P NMR (CD2Cl2) spectrum of complex **1**. δ(ppm) -8.7.



1. Solution 13C NMR (CD2Cl2) spectrum of complex **1**. δ(ppm) 179.5 (Fc*C*OO-); 134.2~129.3 (*Ph*2PCH2P*Ph*2); 117.4 (CH3*C*N); 77.7~69.9 ppm (*Fc*COO-); 27.0 and 26.9 (Ph2P*C*H2PPh2); 2.2 (*C*H3CN).



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1. Solid-state 13C NMR spectrum of complex **1**. δ(ppm) 178.2 (Fc*C*OO-); 129.2 (*Ph*2PCH2P*Ph*2); 121.3 (CH3*C*N); 81.9, 71.7 (*Fc*COO-); 24.6 (Ph2P*C*H2PPh2); 3.1 (*C*H3CN). Notes: The star \*\* peaks are spinning sidebands.



1. The powder XRD pattern of complex **1**.



1. The variable-temperature powder XRD pattern of complex **1** based on phase inversion temperatures in air atmosphere.



1. Cyclic voltammograms of ferrocene (Fc) in dichloromethane solution containing 0.1 М nBu4NPF6 as the supporting electrolyte at 0.1 V·s-1.



1. The molecular structure and atom labelling of [Cu2(μ2-ղ1,ղ1dppm)2(μ2-ղ1,ղ1FcCOO)(CH3CN)]+.

**Tables：**

**Table S1.** Crystal data and structure refinement for **1**.

|  |  |
| --- | --- |
| Chemical formula | C65H59BF4N2O2P4FeCu2 |
| Formula weight | 1293.76 |
| Crystal system | Triclinic |
| Space group | *P*-1 |
| *a*, Ǻ | 12.212(7) |
| *b*, Ǻ | 13.533(8) |
| *c*, Ǻ | 20.361(15) |
| *α*, deg | 79.85(3) |
| *β*, deg | 72.71(4) |
| *γ*, deg | 66.13(2) |
| *V*, Ǻ3 | 2932(3) |
| *Z* | 2 |
| *ρ*calc, g/cm3 | 1.465 |
| *µ*, mm-1 | 1.132 |
| Reflections collected | 73497 |
| Independent reflections | 11584 |
| Rint | 0.0610 |
| Reflections I > 2σ(I) | 11584 |
| Parameters | 732 |
| GOF on F2 | 1.033 |
| *R*1a /*wR*2b (I > 2σ(I)) | 0.0373 / 0.0834 |
| *R*1a /*wR*2b (*all*) | 0.0549 / 0.0909 |

a R1 = [Σ abs(abs(Fo) - abs(Fc))]/ [Σ abs(Fo)]. b *w*R2 = [Σ(*w*(Fo2 - Fc2)2)/ Σ[*w*(Fo2)2]0.5.

**Table S2.** Selected bond lengths [Å] and angles [o] for **1**.

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| --- |
| Bond lengths [Å]  |
| Cu(1)-Cu(2)  | 2.9121(16) | Cu(2)-N(1)  | 2.129(3) |
| Cu(1)-O(1)  | 1.981(2) | Cu(2)-O(2)  | 2.057(2) |
| Cu(1)-P(1)  | 2.2391(14) | Cu(2)-P(2)  | 2.2650(13) |
| Cu(1)-P(3)  | 2.2478(14) | Cu(2)-P(4)  | 2.2665(15) |
| Angles [o] |
| O(1)-Cu(1)-P(1) | 117.87(6) | O(1)-Cu(1)-Cu(2) | 83.59(8) |
| O(1)-Cu(1)-P(3) | 114.30(7) | O(2)-Cu(2)-N(1) | 90.01(10) |
| O(2)-Cu(2)-P(2) | 119.01(7) | O(2)-Cu(2)-P(4) | 112.15(7) |
| O(2)-Cu(2)-Cu(1) | 76.06(7) | N(1)-Cu(2)-P(2) | 103.89(8) |
| N(1)-Cu(2)-P(4) | 97.71(8) | N(1)-Cu(2)-Cu(1) | 165.14(7) |
| P(1)-Cu(1)-P(3) | 127.39(5) | P(2)-Cu(2)-P(4) | 123.75(5) |
| P(1)-Cu(1)-Cu(2) | 93.29(4) | P(2)-Cu(2)-Cu(1) | 87.65(5) |
| P(3)-Cu(1)-Cu(2) | 98.70(4) | P(4)-Cu(2)-Cu(1) | 83.11(4) |