

Supplementary information

Dicarboxamide polymorph derivative for trace level electrochemical sensing of Cu(II) supported with crystal structure and theoretical studies

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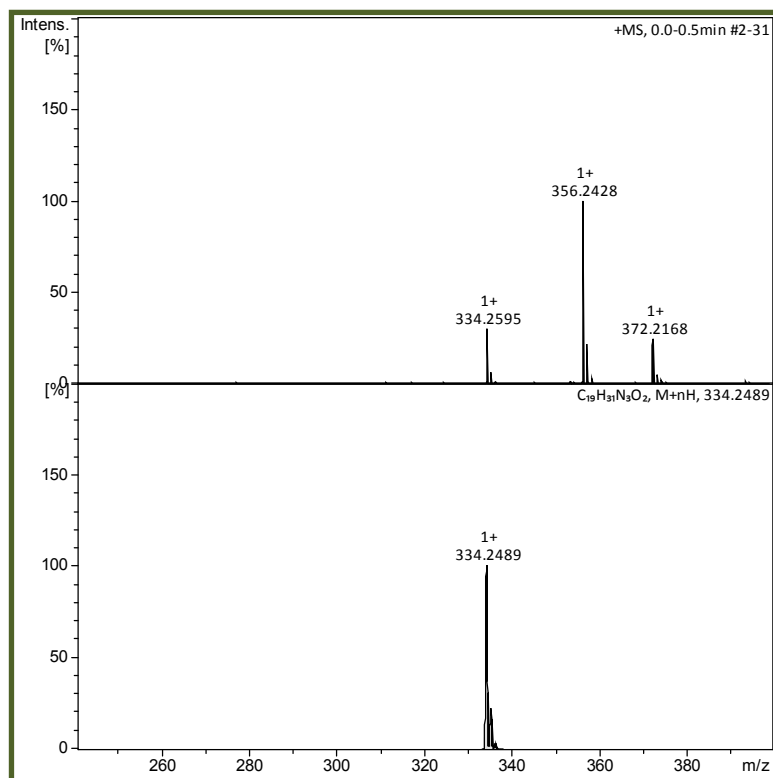


Fig.S3 Mass spectrum of L3.

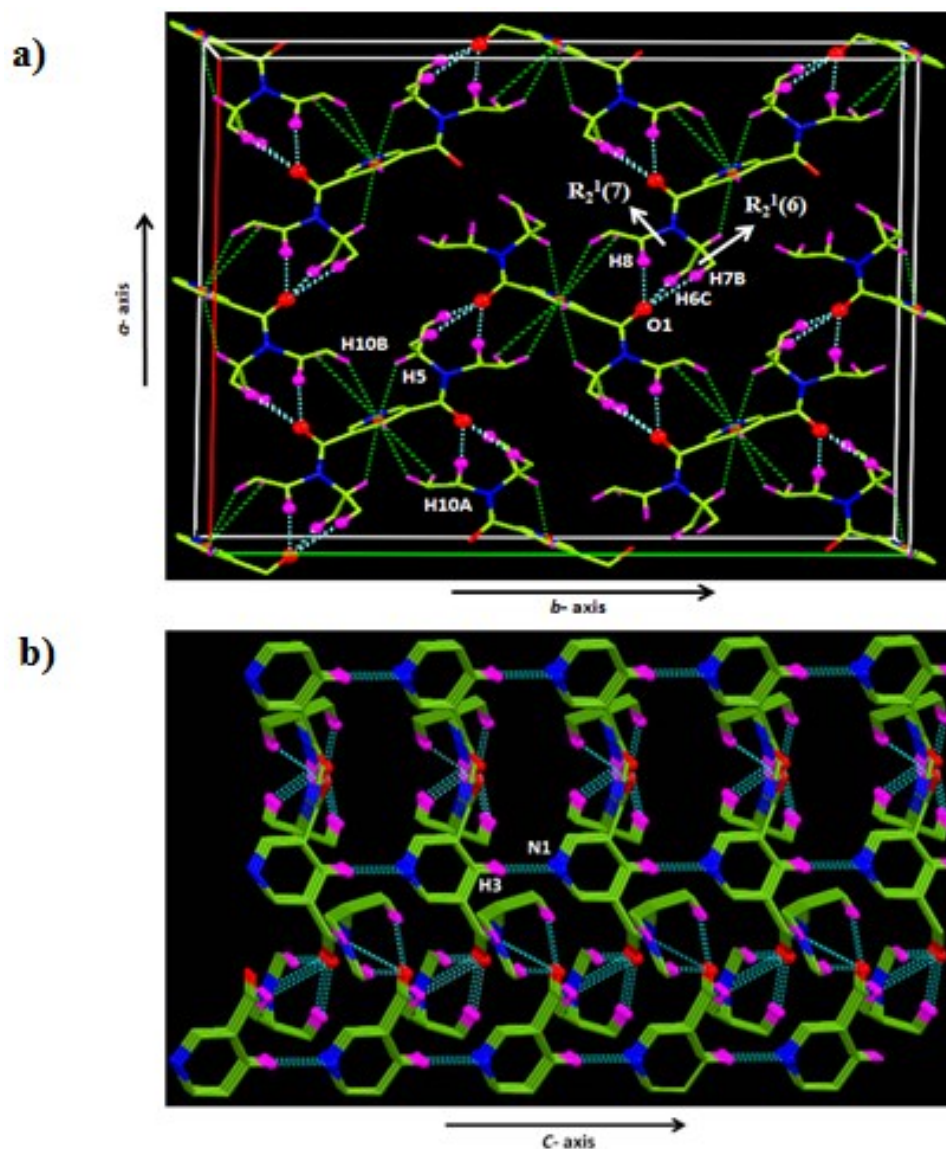


Fig.S4a Showing 2D hydrogen bonded sheet of **L3** running parallel to *ab* plane, **b)** shows how these sheets are connected along *c* axis.

Table S1: Showing various C-H \cdots O/N H-bonding interactions in **L3**.

| D—H \cdots A | A \cdots H/ Å | A \cdots D/ Å | A \cdots H—D/ deg |
|-----------------------------------|-----------------|-----------------|---------------------|
| C9-H9B \cdots O1 | 2.422(2) | 2.981(3) | 115.8 |
| C10-H10C \cdots O1 | 2.453(1) | 3.008(3) | 115.5 |
| C3-H3 \cdots N1 ⁱ | 2.442(3) | 3.392(4) | 180 |
| C3-H3 \cdots N1 ⁱⁱ | 2.442(3) | 3.392(4) | 180 |
| C8-H8 \cdots O1 ⁱⁱⁱ | 2.297(1) | 3.253(2) | 159.7 |
| C6-H6C \cdots O1 ⁱⁱⁱ | 2.835(2) | 3.683(3) | 145.2 |
| C7-H7B \cdots O1 ⁱⁱⁱ | 2.546(1) | 3.467(2) | 156.5 |

Symmetry code : i: $x, y, z-1$, ii: $-x+1, -y, z-1$, iii: $x+1/4, -y-1/4, z-1/4$.

Table S2 : Optimised geometry of Cu(II)-L3 complex at B3LYP-D3/6-31+G(d)-LACVP**

| | | | |
|---|---------------|---------------|---------------|
| C | -1.0210340843 | 2.0589718253 | -0.3059443531 |
| H | -1.8730378257 | 2.6716292848 | -0.5781430383 |
| C | -1.1347847704 | 0.6681632493 | -0.2809913304 |
| C | 0.0062685478 | -0.0872277285 | 0.0006612911 |
| H | -0.0424923443 | -1.1706268245 | 0.0023852370 |
| C | -2.4441270487 | 0.0802568486 | -0.7646536902 |
| C | -2.6678544213 | -1.3475272831 | 1.2932300070 |
| H | -1.9027248050 | -0.6370547750 | 1.6096634313 |
| C | -3.8840096900 | -1.1548719721 | 2.2201556915 |
| H | -4.2755810108 | -0.1370761028 | 2.1498215032 |
| H | -3.5624488674 | -1.3318257929 | 3.2502037533 |
| H | -4.6882386365 | -1.8592827050 | 1.9960032156 |
| C | -2.0907460674 | -2.7726676105 | 1.3890925539 |
| H | -1.2464199245 | -2.9186880323 | 0.7080226165 |
| H | -2.8427074357 | -3.5321538967 | 1.1611627189 |
| H | -1.7456654919 | -2.9428172235 | 2.4126056137 |
| C | -4.1131043339 | -1.7526336563 | -0.7714442343 |
| H | -4.3278124697 | -2.5781024593 | -0.0910745185 |
| C | -3.6457532062 | -2.3435720981 | -2.1132881947 |
| H | -2.7374087323 | -2.9396578817 | -1.9841020464 |
| H | -3.4693233215 | -1.5633616882 | -2.8545422810 |
| H | -4.4329733620 | -3.0033546816 | -2.4874694963 |
| C | -5.3978054059 | -0.9055633111 | -0.9115356357 |
| H | -5.6999090603 | -0.4816782314 | 0.0488271495 |
| H | -6.1964026014 | -1.5665189144 | -1.2595890479 |
| H | -5.2592598682 | -0.1035881368 | -1.6358377449 |
| N | 0.1344090830 | 2.6914470204 | -0.0046964577 |
| N | -3.0115483518 | -1.0014319341 | -0.1070841432 |

| | | | |
|----|---------------|---------------|---------------|
| O | -2.9460916463 | 0.5820584077 | -1.7633482377 |
| C | 1.2268622766 | 1.9567237722 | 0.3001173854 |
| H | 2.1310428155 | 2.4899289769 | 0.5709370131 |
| C | 1.2116359994 | 0.5618321381 | 0.2802931464 |
| C | 2.4575156705 | -0.1460241867 | 0.7700352778 |
| C | 2.5626117706 | -1.5774483220 | -1.2940099599 |
| H | 1.8733178322 | -0.7935715340 | -1.6128320778 |
| C | 3.8035297989 | -1.4965315368 | -2.2048285035 |
| H | 4.2896732653 | -0.5213756127 | -2.1227786898 |
| H | 3.4799623851 | -1.6362690244 | -3.2399420155 |
| H | 4.5337780690 | -2.2758154622 | -1.9753663800 |
| C | 1.8523302926 | -2.9401797213 | -1.4095182398 |
| H | 0.9890479622 | -3.0103904603 | -0.7404096745 |
| H | 2.5247904244 | -3.7704433827 | -1.1802641241 |
| H | 1.5053266309 | -3.0681550454 | -2.4385282760 |
| C | 3.9362952338 | -2.1363088073 | 0.7845381735 |
| H | 4.0743347778 | -2.9773225052 | 0.1035210448 |
| C | 3.3970266687 | -2.6795998768 | 2.1196058096 |
| H | 2.4350335363 | -3.1814376693 | 1.9787242253 |
| H | 3.2913589961 | -1.8869804738 | 2.8612544025 |
| H | 4.1098095962 | -3.4156160887 | 2.5007459783 |
| C | 5.2982493079 | -1.4236618965 | 0.9417927810 |
| H | 5.6516202404 | -1.0294614765 | -0.0135885809 |
| H | 6.0222355602 | -2.1630270633 | 1.2952484751 |
| H | 5.2336518954 | -0.6141129539 | 1.6679065613 |
| N | 2.9229292436 | -1.2758124995 | 0.1123993580 |
| O | 2.9993869980 | 0.3035411883 | 1.7723167934 |
| Cu | 0.2251606745 | 4.6486522881 | -0.0177082555 |

Table S3 : Optimised geometry of L3 at B3LYP-D3/6-31+G(d)

| | | | |
|---|---------------|---------------|---------------|
| C | -1.0210340843 | 2.0589718253 | -0.3059443531 |
| H | -1.8730378257 | 2.6716292848 | -0.5781430383 |
| C | -1.1347847704 | 0.6681632493 | -0.2809913304 |
| C | 0.0062685478 | -0.0872277285 | 0.0006612911 |
| H | -0.0424923443 | -1.1706268245 | 0.0023852370 |
| C | -2.4441270487 | 0.0802568486 | -0.7646536902 |
| C | -2.6678544213 | -1.3475272831 | 1.2932300070 |
| H | -1.9027248050 | -0.6370547750 | 1.6096634313 |
| C | -3.8840096900 | -1.1548719721 | 2.2201556915 |
| H | -4.2755810108 | -0.1370761028 | 2.1498215032 |
| H | -3.5624488674 | -1.3318257929 | 3.2502037533 |
| H | -4.6882386365 | -1.8592827050 | 1.9960032156 |
| C | -2.0907460674 | -2.7726676105 | 1.3890925539 |
| H | -1.2464199245 | -2.9186880323 | 0.7080226165 |
| H | -2.8427074357 | -3.5321538967 | 1.1611627189 |
| H | -1.7456654919 | -2.9428172235 | 2.4126056137 |
| C | -4.1131043339 | -1.7526336563 | -0.7714442343 |
| H | -4.3278124697 | -2.5781024593 | -0.0910745185 |
| C | -3.6457532062 | -2.3435720981 | -2.1132881947 |
| H | -2.7374087323 | -2.9396578817 | -1.9841020464 |
| H | -3.4693233215 | -1.5633616882 | -2.8545422810 |
| H | -4.4329733620 | -3.0033546816 | -2.4874694963 |
| C | -5.3978054059 | -0.9055633111 | -0.9115356357 |
| H | -5.6999090603 | -0.4816782314 | 0.0488271495 |
| H | -6.1964026014 | -1.5665189144 | -1.2595890479 |
| H | -5.2592598682 | -0.1035881368 | -1.6358377449 |
| N | 0.1344090830 | 2.6914470204 | -0.0046964577 |
| N | -3.0115483518 | -1.0014319341 | -0.1070841432 |
| O | -2.9460916463 | 0.5820584077 | -1.7633482377 |
| C | 1.2268622766 | 1.9567237722 | 0.3001173854 |
| H | 2.1310428155 | 2.4899289769 | 0.5709370131 |

| | | | |
|---|--------------|---------------|---------------|
| C | 1.2116359994 | 0.5618321381 | 0.2802931464 |
| C | 2.4575156705 | -0.1460241867 | 0.7700352778 |
| C | 2.5626117706 | -1.5774483220 | -1.2940099599 |
| H | 1.8733178322 | -0.7935715340 | -1.6128320778 |
| C | 3.8035297989 | -1.4965315368 | -2.2048285035 |
| H | 4.2896732653 | -0.5213756127 | -2.1227786898 |
| H | 3.4799623851 | -1.6362690244 | -3.2399420155 |
| H | 4.5337780690 | -2.2758154622 | -1.9753663800 |
| C | 1.8523302926 | -2.9401797213 | -1.4095182398 |
| H | 0.9890479622 | -3.0103904603 | -0.7404096745 |
| H | 2.5247904244 | -3.7704433827 | -1.1802641241 |
| H | 1.5053266309 | -3.0681550454 | -2.4385282760 |
| C | 3.9362952338 | -2.1363088073 | 0.7845381735 |
| H | 4.0743347778 | -2.9773225052 | 0.1035210448 |
| C | 3.3970266687 | -2.6795998768 | 2.1196058096 |
| H | 2.4350335363 | -3.1814376693 | 1.9787242253 |
| H | 3.2913589961 | -1.8869804738 | 2.8612544025 |
| H | 4.1098095962 | -3.4156160887 | 2.5007459783 |
| C | 5.2982493079 | -1.4236618965 | 0.9417927810 |
| H | 5.6516202404 | -1.0294614765 | -0.0135885809 |
| H | 6.0222355602 | -2.1630270633 | 1.2952484751 |
| H | 5.2336518954 | -0.6141129539 | 1.6679065613 |
| N | 2.9229292436 | -1.2758124995 | 0.1123993580 |
| O | 2.9993869980 | 0.3035411883 | 1.7723167934 |