<Electronic Supplementary Information>

# M(II) effect on encapsulation of guests into series of $M_3L_2$ chiral cages: Enantio-recognition

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## **Table S1** Crystallographic data

| | $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ | $[(Me_2CO)@Cu_3(s,r\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ | $[(Me_2CO)(H_2O)@Zn_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ |
|---|---|---|---|
| Formula | $C_{132}H_{156}Cl_6N_{12}Ni_3O_{62}$ | $C_{132}H_{150}Cl_6Cu_3N_{12}O_{59}$ | $C_{132}H_{156}Cl_6N_{12}O_{62}Zn_3$ |
| $M_w$ | 3291.51 | 3251.95 | 3311.49 |
| Cryst. sys. | Orthorhombic | Orthorhombic | Orthorhombic |
| Space group | $P2_12_12$ | $P2_12_12$ | $P2_12_12$ |
| $a$ (Å) | 23.168(5) | 10.6097(2) | 23.173(3) |
| $b$ (Å) | 24.785(5) | 24.982(5) | 24.840(3) |
| $c$ (Å) | 14.620(3) | 14.522(3) | 14.539(2) |
| $V$ (Å$^3$) | 8395(3) | 8356(3) | 8369(2) |
| $Z$ | 2 | 2 | 2 |
| $\rho$ (g cm$^{-3}$) | 1.302 | 1.292 | 1.314 |
| $\mu$ (mm$^{-1}$) | 0.492 | 0.535 | 0.610 |
| F(000) | 3428 | 3374 | 3440 |
| $R_{int}$ | 0.0522 | 0.0544 | 0.1033 |
| GoF on $F^2$ | 1.158 | 1.058 | 1.020 |
| $R_1$ [$I$>2$\sigma$($I$)][a] | 0.0611 | 0.0518 | 0.0668 |
| $wR_2$ (all data)[b] | 0.2035 | 0.1609 | 0.2141 |
| Absolute structure parameter | 0.023(3) | 0.010(3) | 0.032(5) |
| | $[(Me_2CO)(H_2O)@Ni_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ | $[(Me_2CO)@Cu_3(r,s\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ | $[(Me_2CO)(H_2O)@Zn_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ |
| Formula | $C_{132}H_{156}Cl_6N_{12}Ni_3O_{62}$ | $C_{264}H_{300}Cl_{12}Cu_6N_{24}O_{118}$ | $C_{132}H_{156}Cl_6N_{12}O_{62}Zn_3$ |
| $M_w$ | 3291.51 | 6503.90 | 3311.49 |
| Cryst. sys. | Orthorhombic | Orthorhombic | Orthorhombic |
| Space group | $P2_12_12$ | $P2_12_12$ | $P2_12_12$ |
| $a$ (Å) | 23.136(5) | 22.963(5) | 23.292(5) |
| $b$ (Å) | 24.872(5) | 24.980(5) | 24.799(5) |
| $c$ (Å) | 14.593(3) | 14.527(3) | 14.573(3) |
| $V$ (Å$^3$) | 8397(3) | 8333(3) | 8418(3) |
| $Z$ | 2 | 1 | 2 |
| $\rho$ (g cm$^{-3}$) | 1.302 | 1.296 | 1.307 |
| $\mu$ (mm$^{-1}$) | 0.492 | 0.536 | 0.649 |
| F(000) | 3428 | 3374 | 3440 |
| $R_{int}$ | 0.0430 | 0.0460 | 0.0834 |
| GoF on $F^2$ | 1.089 | 0.995 | 0.980 |
| $R_1$ [$I$>2$\sigma$($I$)][a] | 0.0607 | 0.0592 | 0.1148 |
| $wR_2$ (all data)[b] | 0.1865 | 0.1765 | 0.3346 |
| Absolute structure parameter | 0.024(3) | 0.021(5) | 0.073(7) |

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR_2 = (\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2])^{1/2}$

**Table S1** (Continued)

| | $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot6((S)\text{-}2\text{-}BuOH)$ | $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot6((R)\text{-}2\text{-}BuOH)$ |
|---|---|---|
| Formula | $C_{135}H_{174}Cl_6N_{12}Ni_3O_{61}$ | $C_{135}H_{174}Cl_6N_{12}Ni_3O_{61}$ |
| $M_w$ | 3329.68 | 3329.68 |
| Cryst. sys. | Orthorhombic | Orthorhombic |
| Space group | $P2_12_12$ | $P2_12_12$ |
| $a$ (Å) | 23.205(5) | 23.225(5) |
| $b$ (Å) | 24.806(5) | 24.677(5) |
| $c$ (Å) | 14.483(3) | 14.453(3) |
| $V$ (Å$^3$) | 8337(3) | 8283(3) |
| $Z$ | 2 | 2 |
| $\rho$ (g cm$^{-3}$) | 1.326 | 1.335 |
| $\mu$ (mm$^{-1}$) | 0.496 | 0.0479 |
| F(000) | 3484 | 3484 |
| $R_{int}$ | 0.0729 | 0.0544 |
| GoF on $F^2$ | 1.093 | 1.184 |
| $R_1$ $[I>2\sigma(I)]^a$ | 0.0767 | 0.0656 |
| $wR_2$ (all data)$^b$ | 0.2580 | 0.2253 |
| Absolute structure parameter | 0.030(3) | 0.027(3) |

| | $[(Me_2CO)(H_2O)@Ni_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot6((S)\text{-}2\text{-}BuOH)$ | $[(Me_2CO)(H_2O)@Ni_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot6((R)\text{-}2\text{-}BuOH)$ |
|---|---|---|
| Formula | $C_{135}H_{174}Cl_6N_{12}Ni_3O_{61}$ | $C_{135}H_{174}Cl_6N_{12}Ni_3O_{61}$ |
| $M_w$ | 3329.68 | 3329.68 |
| Cryst. sys. | Orthorhombic | Orthorhombic |
| Space group | $P2_12_12$ | $P2_12_12$ |
| $a$ (Å) | 23.201(5) | 23.255(5) |
| $b$ (Å) | 24.714(5) | 24.745(5) |
| $c$ (Å) | 14.446(3) | 14.510(3) |
| $V$ (Å$^3$) | 8283(3) | 8350(3) |
| $Z$ | 2 | 2 |
| $\rho$ (g cm$^{-3}$) | 1.335 | 1.324 |
| $\mu$ (mm$^{-1}$) | 0.499 | 0.495 |
| F(000) | 3484 | 3484 |
| $R_{int}$ | 0.0423 | 0.0522 |
| GoF on $F^2$ | 1.131 | 1.019 |
| $R_1$ $[I>2\sigma(I)]^a$ | 0.0744 | 0.0615 |
| $wR_2$ (all data)$^b$ | 0.2467 | 0.1882 |
| Absolute structure parameter | 0.030(3) | 0.020(3) |

$^aR_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $^bwR_2 = (\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2])^{1/2}$

**Table S2** Selected bond length (Å) and angle (°)

| [(Me$_2$CO)(H$_2$O)@Ni$_3$(*s*,*r*-L)$_2$(H$_2$O)$_{11}$](ClO$_4$)$_6$·7Me$_2$CO | | [(Me$_2$CO)@Cu$_3$(*s*,*r*-L)$_2$(H$_2$O)$_9$](ClO$_4$)$_6$·7Me$_2$CO | | [(Me$_2$CO)(H$_2$O)@Zn$_3$(*s*,*r*-L)$_2$(H$_2$O)$_{11}$](ClO$_4$)$_6$·7Me$_2$CO | |
|---|---|---|---|---|---|
| Ni(1)-N(3) | 2.088(4) | Cu(1)-N(6) | 1.978(4) | Zn(1)-N(1A) | 2.132(7) |
| Ni(1)-N(5)$^{\#1}$ | 2.090(4) | Cu(2)$^{\#1}$-N(1) | 1.997(4) | Zn(1)-N(4A)$^{\#1}$ | 2.110(7) |
| Ni(2)-N(1) | 2.077(4) | Cu(2)-N(4) | 1.999(4) | Zn(2)-N(6A) | 2.072(7) |
| Ni(1)-O(10) | 2.027(5) | Cu(1)-O(2A) | 1.978(3) | Zn(1)-O(13) | 2.086(7) |
| Ni(1)-O(11) | 2.029(5) | Cu(1)-O(1A) | 2.354(5) | Zn(1)-O(11) | 2.087(6) |
| Ni(1)-O(12) | 2.057(5) | Cu(2)-O(3A) | 2.364(2) | Zn(1)-O(14) | 2.094(7) |
| Ni(1)-O(17) | 2.093(9) | Cu(2)-O(5A) | 1.978(4) | Zn(2)-O(15) | 2.093(6) |
| Ni(2)-O(15) | 2.049(5) | Cu(2)-O(4A) | 2.227(5) | Zn(2)-O(16) | 2.135(8) |
| Ni(2)-O(14) | 2.082(5) | | | Zn(2)-O(17) | 2.30(1) |
| | | N(6)-Cu(1)-N(6)$^{\#1}$ | 175.7(2) | | |
| N(3)-Ni(1)-N(5)$^{\#1}$ | 176.5(2) | N(1)$^{\#1}$-Cu(2)-N(4) | 171.6(2) | N(4A)$^{\#1}$-Zn(1)-N(1A) | 175.0(3) |
| N(1)-Ni(2)-N(1)$^{\#1}$ | 177.6(2) | N(6)-Cu(1)-O(2A) | 88.4(2) | N(6A)$^{\#1}$-Zn(2)-N(6A) | 176.2(4) |
| O(10)-Ni(1)-N(3) | 88.4(2) | N(6)$^{\#1}$-Cu(1)-O(2A) | 91.6(2) | O(13)-Zn(1)-N(1A) | 93.8(3) |
| O(11)-Ni(1)-N(3) | 89.4(2) | N(6)-Cu(1)-O(1A) | 92.2(1) | O(11)-Zn(1)-N(1A) | 93.0(2) |
| O(12)-Ni(1)-N(3) | 91.0(2) | O(3A)-Cu(2)-N(1)$^{\#1}$ | 90.0(2) | O(14)-Zn(1)-N(1A) | 88.0(3) |
| N(3)-Ni(1)-O(17) | 94.3(3) | O(5A)-Cu(2)-N(1)$^{\#1}$ | 88.1(2) | N(4A)$^{\#1}$-Zn(1)-O(12) | 85.6(3) |
| O(15)-Ni(2)-N(1) | 92.3(2) | O(3A)-Cu(2)-N(4) | 89.8(2) | N(6A)-Zn(2)-O(15) | 87.2(2) |
| O(15)$^{\#1}$-Ni(2)-N(1) | 87.8(2) | O(5A)-Cu(2)-N(4) | 90.5(2) | N(6A)-Zn(2)-O(16) | 91.9(2) |
| N(1)-Ni(2)-O(14) | 91.2(1) | N(1)$^{\#1}$-Cu(2)-O(4A) | 95.2(2) | N(6A)-Zn(2)-O(17) | 88.1(2) |
| N(1)-Ni(2)-O(1B) | 88.8(1) | N(4)-Cu(2)-O(4A) | 93.1(2) | | |
| $^{\#1}$ $x+1, -y+1, z$ | | $^{\#1}$ $-x+1, -y+1, z$ | | $^{\#1}$ $-x+1, -y+1, z$ | |

| [(Me$_2$CO)(H$_2$O)@Ni$_3$(*r*,*s*-L)$_2$(H$_2$O)$_{11}$](ClO$_4$)$_6$·7Me$_2$CO | | [(Me$_2$CO)@Cu$_3$(*r*,*s*-L)$_2$(H$_2$O)$_9$](ClO$_4$)$_6$·7Me$_2$CO | | [(Me$_2$CO)(H$_2$O)@Zn$_3$(*r*,*s*-L)$_2$(H$_2$O)$_{11}$](ClO$_4$)$_6$·7Me$_2$CO | |
|---|---|---|---|---|---|
| Ni(1)-N(5)$^{\#1}$ | 2.090(5) | Cu(1)-N(4) | 1.986(6) | Zn(1)-N(43) | 2.122(6) |
| Ni(1)-N(3) | 2.094(5) | Cu(2)-N(6)$^{\#1}$ | 1.982(6) | Zn(1)-N(64)$^{\#1}$ | 2.104(7) |
| Ni(2)-N(1) | 2.062(5) | Cu(1)-O(4A) | 2.001(4) | Zn(2)-N(22) | 2.097(6) |
| Ni(1)-O(15) | 2.037(5) | Cu(1)-O(5A) | 2.381(6) | Zn(1)-O(73) | 2.09(1) |
| Ni(1)-O(13) | 2.057(4) | Cu(2)-O(3A) | 1.949(5) | Zn(1)-O(72) | 2.10(1) |
| Ni(1)-O(16) | 2.058(5) | Cu(2)-O(1A) | 1.960(6) | Zn(1)-O(70) | 2.16(1) |
| Ni(2)-O(10) | 2.065(5) | Cu(2)-O(2A) | 2.248(6) | Zn(2)-O(74) | 2.11(1) |
| | | | | Zn(2)-O(2) | 2.11(2) |
| N(5)$^{\#1}$-Ni(1)-N(3) | 176.5(2) | N(4)-Cu(1)-N(4)$^{\#1}$ | 174.9(3) | Zn(2)-O(3) | 2.30(2) |
| N(1)-Ni(2)-N(1)$^{\#1}$ | 177.7(2) | N(6)$^{\#1}$-Cu(2)-N(2) | 172.6(2) | | |
| O(15)-Ni(1)-N(5)#1 | 89.3(2) | N(4)-Cu(1)-O(4A) | 88.3(2) | N(64)$^{\#1}$-Zn(1)-N(43) | 175.1(4) |
| O(13)-Ni(1)-N(5)#1 | 91.45(17) | N(4)$^{\#1}$-Cu(1)-O(4A) | 91.6(2) | N(22)$^{\#1}$-Zn(2)-N(22) | 176.0(5) |
| O(16)-Ni(1)-N(5)#1 | 93.35(19) | N(4)-Cu(1)-O(5A) | 92.5(2) | O(73)-Zn(1)-N(43) | 87.8(4) |
| O(15)-Ni(1)-N(3) | 87.91(19) | O(3A)-Cu(2)-N(6)$^{\#1}$ | 90.6(2) | O(71)-Zn(1)-N(43) | 91.3(4) |
| O(13)-Ni(1)-N(3) | 91.11(18) | O(1A)-Cu(2)-N(6)$^{\#1}$ | 87.9(2) | O(72)-Zn(1)-N(43) | 87.9(4) |
| O(16)-Ni(1)-N(3) | 88.85(18) | O(3A)-Cu(2)-N(2) | 89.3(2) | N(43)-Zn(1)-O(70) | 86.6(4) |
| N(1)-Ni(2)-O(10) | 91.16(12) | O(1A)-Cu(2)-N(2) | 90.8(2) | N(22)-Zn(2)-O(74) | 87.7(4) |
| O(11)-Ni(2)-O(1B) | 90.32(19) | N(6)$^{\#1}$-Cu(2)-O(2A) | 94.4(2) | N(22)-Zn(2)-O(2) | 92.0(2) |
| N(1)-Ni(2)-O(1B) | 88.84(12) | N(2)-Cu(2)-O(2A) | 92.8(2) | N(22)-Zn(2)-O(3) | 88.0(2) |
| $^{\#1}$ $-x+1, -y+1, z$ | | $^{\#1}$ $-x+1,-y+1, z$ | | $^{\#1}$ $-x+1, -y+1, z$ | |

**Table S3** Solubility of the ligands and the complexes in some selected solvents

| **Sample** | L | $Ni_3L_2$ | $Cu_3L_2$ | $Zn_3L_2$ |
|---|---|---|---|---|
| $H_2O$ | IS | SS | SS | SS |
| EtOH | IS | S | S | S |
| $CH_3CN$ | S | S | S | S |
| $Me_2CO$ | S | SS | SS | SS |
| $CHCl_3$ | S | IS | IS | IS |
| $CH_2Cl_2$ | S | IS | IS | IS |
| $Me_2SO$ | S | S | S | S |
| DMF | S | S | S | S |

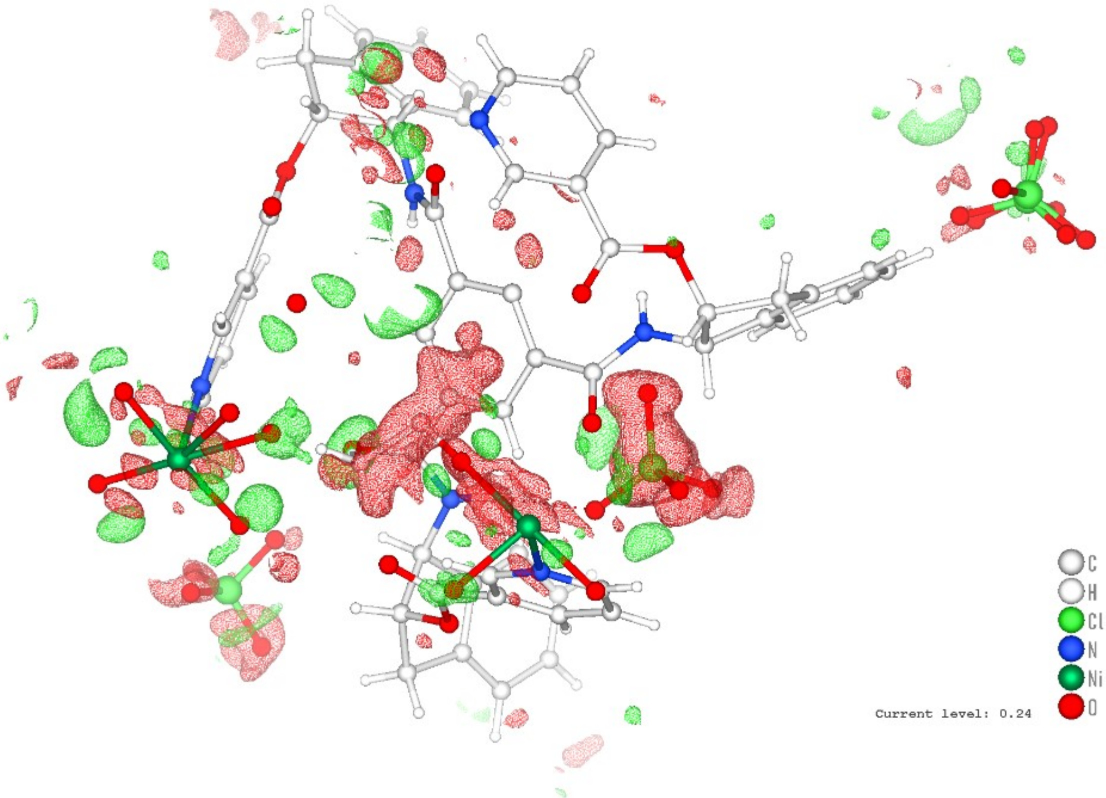
S = Soluble; SS = Sparingly soluble; IS = Insoluble

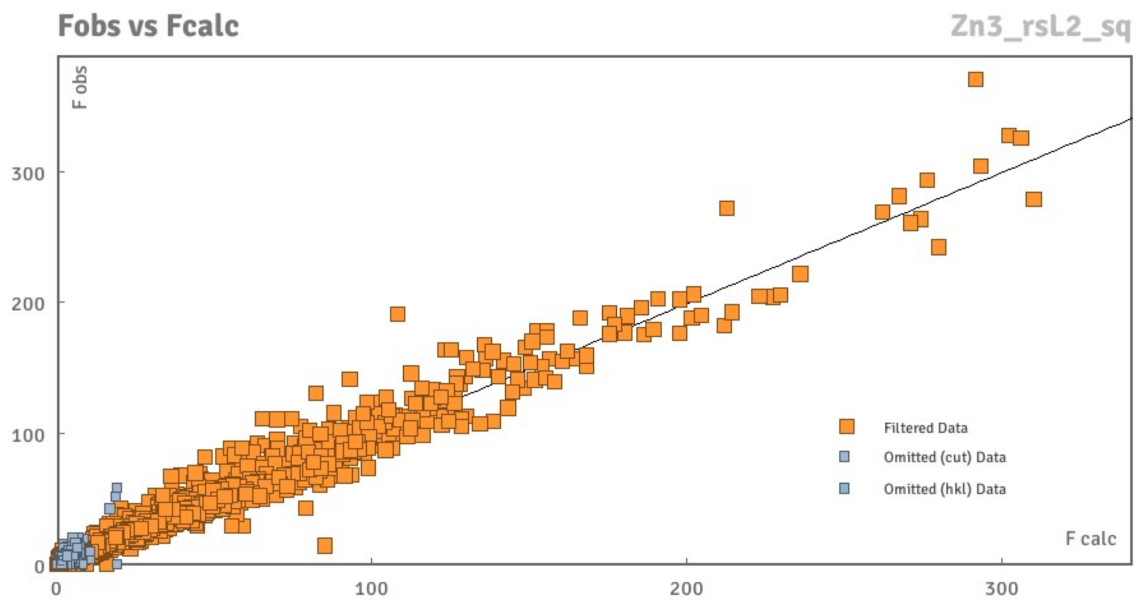
$Ni_3L_2$ = $[(Me_2CO)(H_2O)@Ni_3(s,r\text{- or }r,s\text{-L})_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$

$Cu_3L_2$ = $[(Me_2CO)@Cu_3(s,r\text{- or }r,s\text{- L})_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$

$Zn_3L_2$ = $[(Me_2CO)(H_2O)@Zn_3(s,r\text{- or }r,s\text{-L})_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$

## Crystallographic data problems




All crystals showed low crystallinity as well as sensitivity to the aerobic condition, and the synchrotron can measure data by one axis only. Insufficient data make several problems:

1. The perchlorate anions seems to over-assigned (top figure).

2. Fobs vs Fcalc plot of Zn3_rsL2_sq was not good (bottom figure).

So we confirmed the cage structures using different methods (NMR, IR, CD, and Mass). And the chiral butanol exchanged data is only used for interaction modeling for DFT calculation.

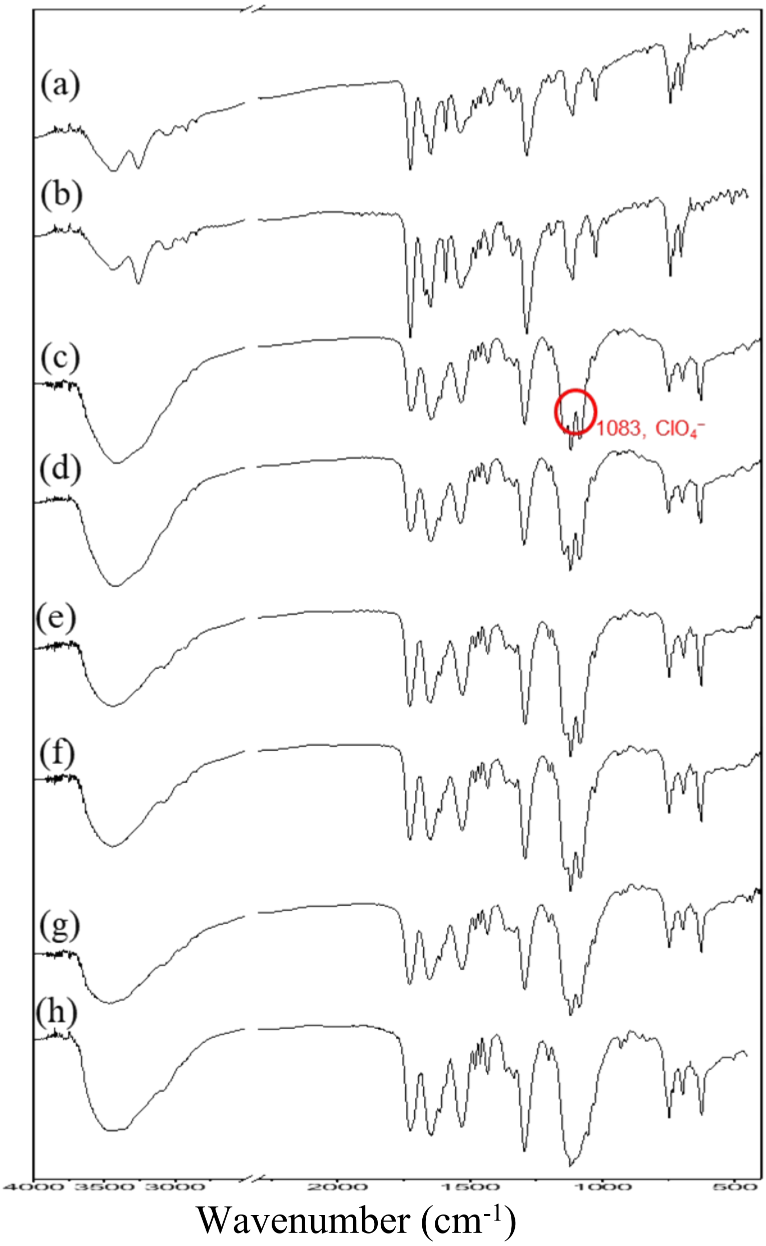



**Fig. S1** IR spectra of *s*,*r*-L (a), *r*,*s*-L (b), $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (c), $[(Me_2CO)(H_2O)@Ni_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (d), $[(Me_2CO)@Cu_3(s,r\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ (e), $[(Me_2CO)@Cu_3(r,s\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ (f), $[(Me_2CO)(H_2O)@Zn_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (g), and $[(Me_2CO)(H_2O)@Zn_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (h).

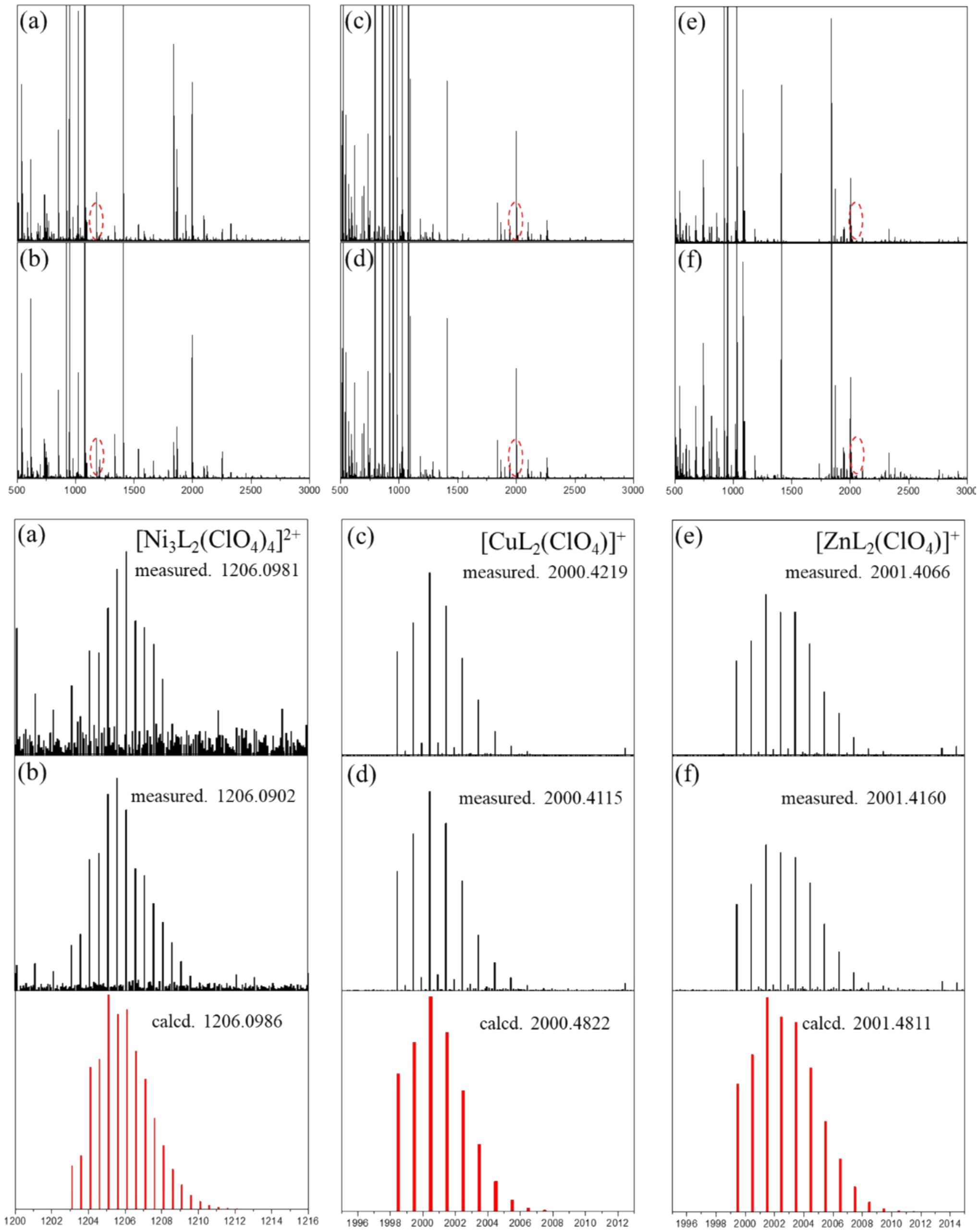



**Fig. S2** ESI-Mass data of $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6 \cdot 7Me_2CO$ (a), $[(Me_2CO)(H_2O)@Ni_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6 \cdot 7Me_2CO$ (b), $[(Me_2CO)@Cu_3(s,r\text{-}L)_2(H_2O)_9](ClO_4)_6 \cdot 7Me_2CO$ (c), $[(Me_2CO)@Cu_3(r,s\text{-}L)_2(H_2O)_9](ClO_4)_6 \cdot 7Me_2CO$ (d), $[(Me_2CO)(H_2O)@Zn_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6 \cdot 7Me_2CO$ (e), and $[(Me_2CO)(H_2O)@Zn_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6 \cdot 7Me_2CO$ (f).

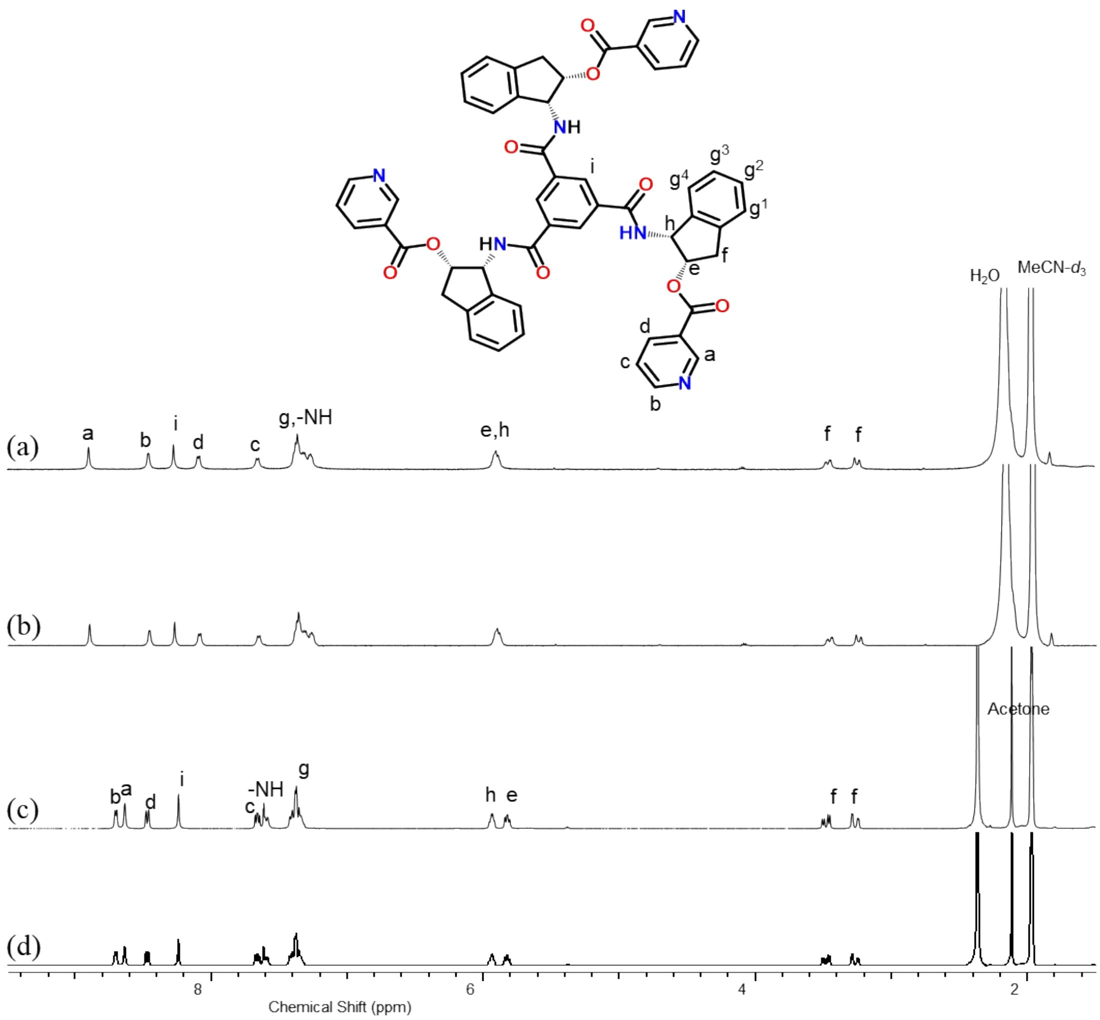



**Fig. S3** $^{1}$H NMR spectra of *s*,*r*-L (a), *r*,*s*-L (b), [$(Me_2CO)(H_2O)@Zn_3$(*s*,*r*-L)$_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (c), and [$(Me_2CO)(H_2O)@Zn_3$(*r*,*s*-L)$_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (d) in MeCN-$d_3$.

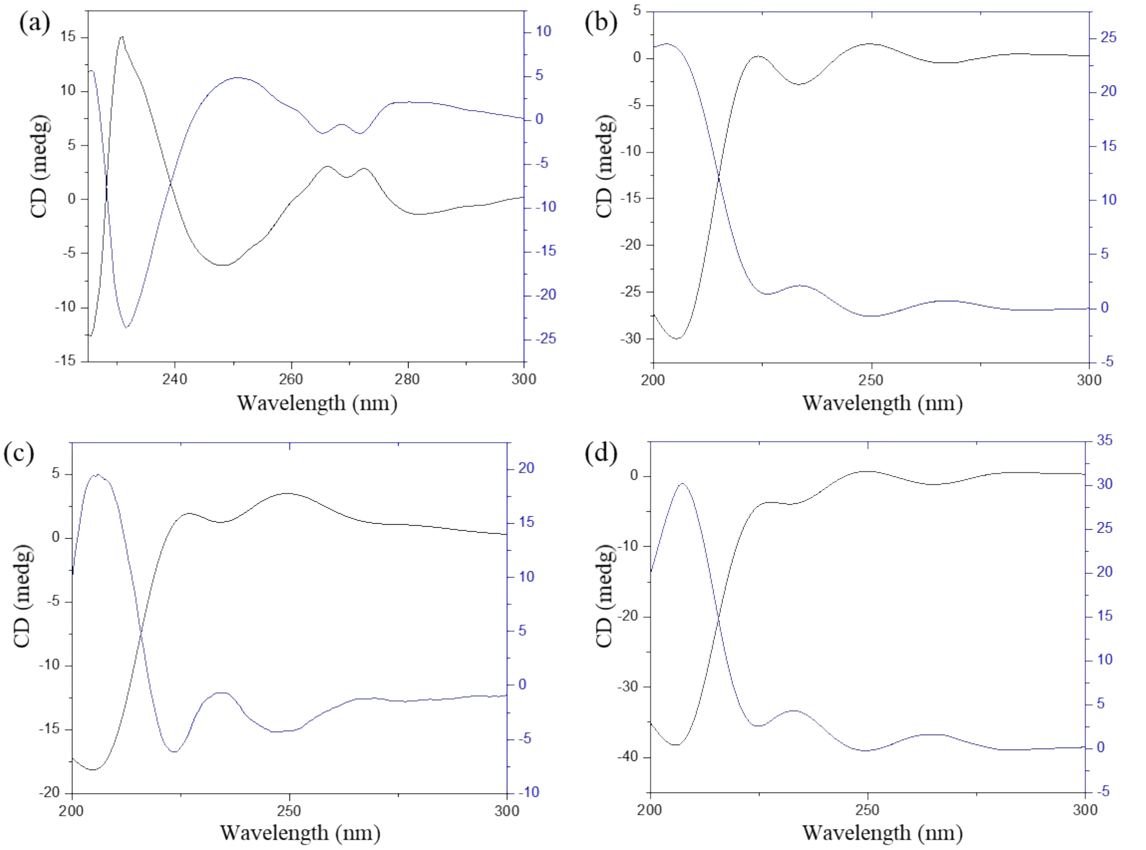



**Fig. S4** CD spectra for *s*,*r*-L (black line) and *r*,*s*-L (blue line) (a), $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (black line), $[(Me_2CO)(H_2O)@Ni_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (blue line) (b), $[(Me_2CO)@Cu_3(s,r\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ (black line), $[(Me_2CO)@Cu_3(r,s\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ (blue line) (c), $[(Me_2CO)(H_2O)@Zn_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (black line), and $[(Me_2CO)(H_2O)@Zn_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (blue line) (d).

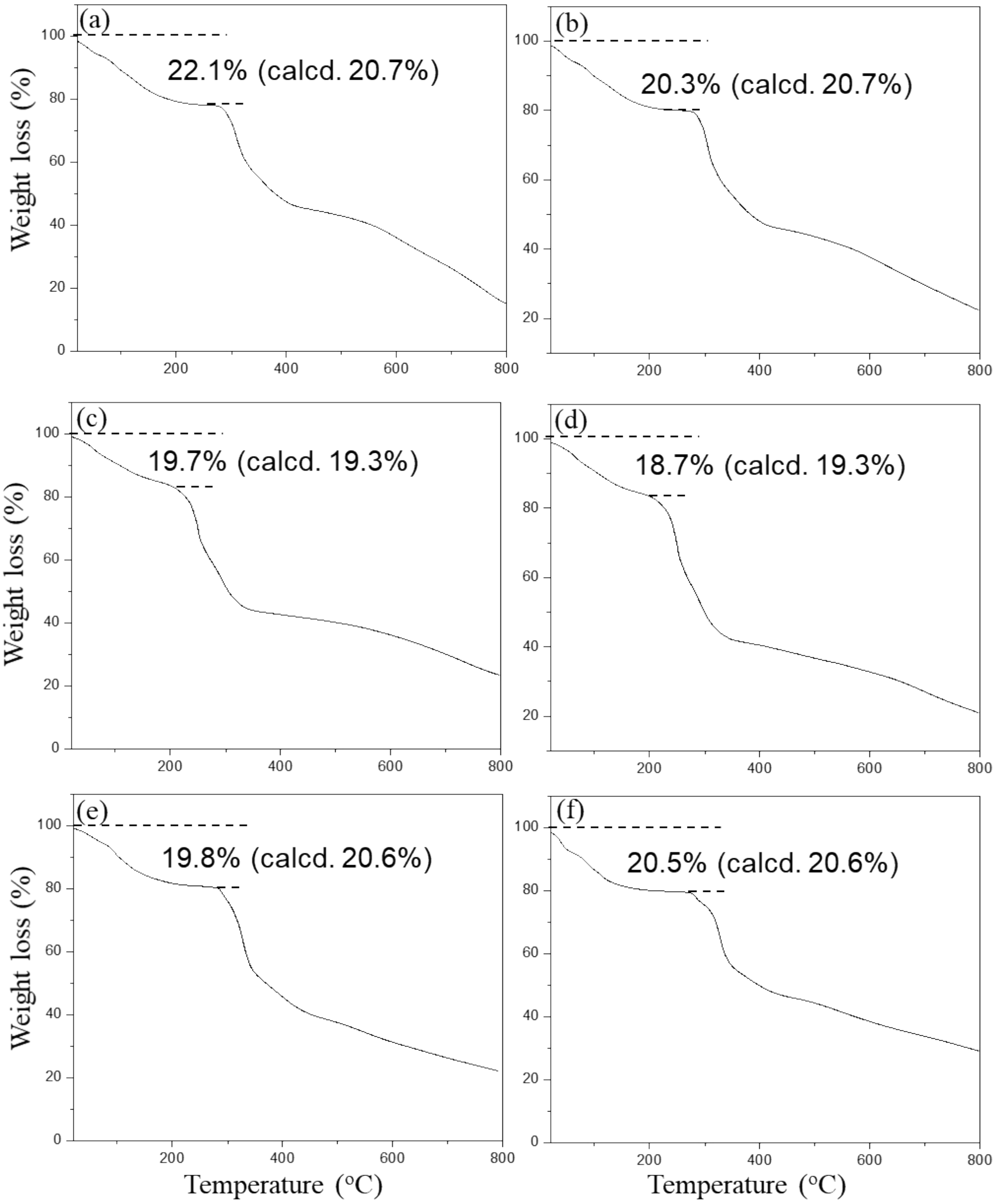



**Fig. S5** TG curves for $[(Me_2CO)(H_2O)@Ni_3(\mathit{s,r}\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot7Me_2CO$ (a), $[(Me_2CO)(H_2O)@Ni_3(\mathit{r,s}\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot7Me_2CO$ (b), $[(Me_2CO)@Cu_3(\mathit{s,r}\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot7Me_2CO$ (c), $[(Me_2CO)@Cu_3(\mathit{r,s}\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot7Me_2CO$ (d), $[(Me_2CO)(H_2O)@Zn_3(\mathit{s,r}\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot7Me_2CO$ (e), and $[(Me_2CO)(H_2O)@Zn_3(\mathit{r,s}\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot7Me_2CO$ (f).

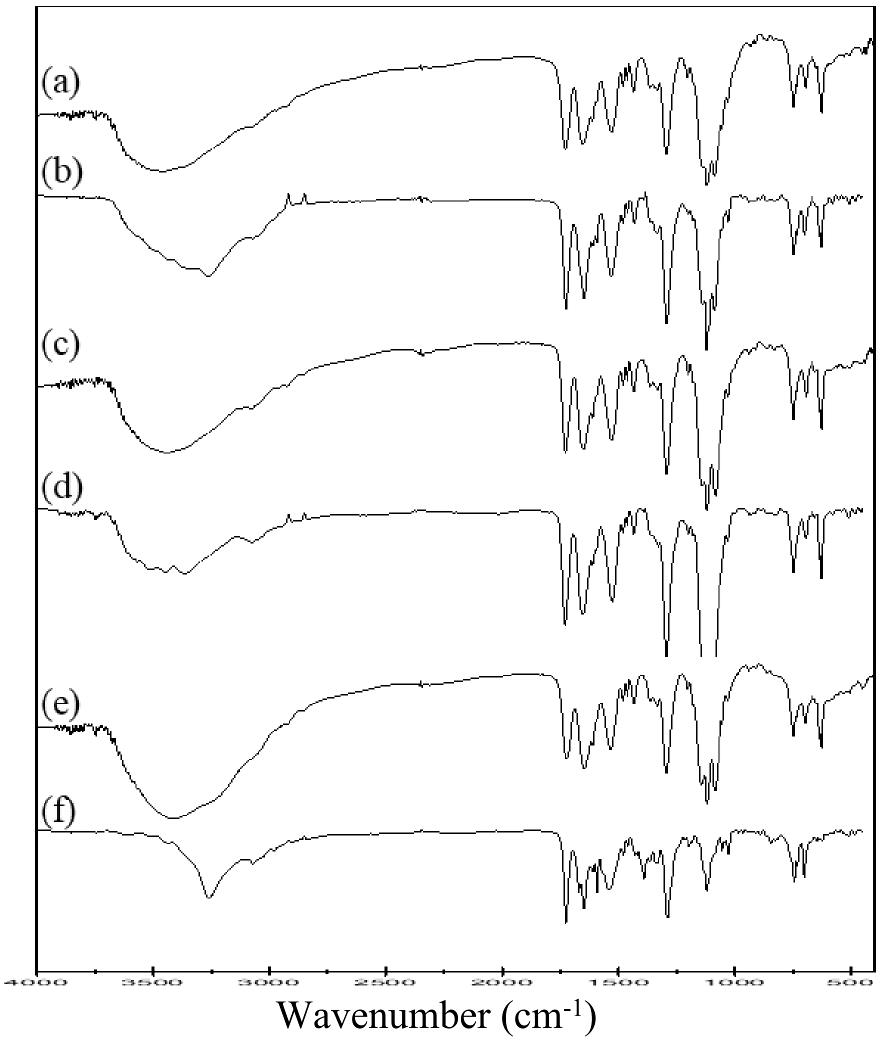



**Fig. S6** IR spectra of $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6{\cdot}7Me_2CO$ (a), $[(Me_2CO)@Cu_3(s,r\text{-}L)_2(H_2O)_9](ClO_4)_6{\cdot}7Me_2CO$ (c), and $[(Me_2CO)(H_2O)@Zn_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6{\cdot}7Me_2CO$ (e). IR spectra of dispersed in EtOH by sonication for 4 h and drop-casted $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6{\cdot}7Me_2CO$ (b), $[(Me_2CO)@Cu_3(s,r\text{-}L)_2(H_2O)_9](ClO_4)_6{\cdot}7Me_2CO$ (d), and $[(Me_2CO)(H_2O)@Zn_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6{\cdot}7Me_2CO$ (f).

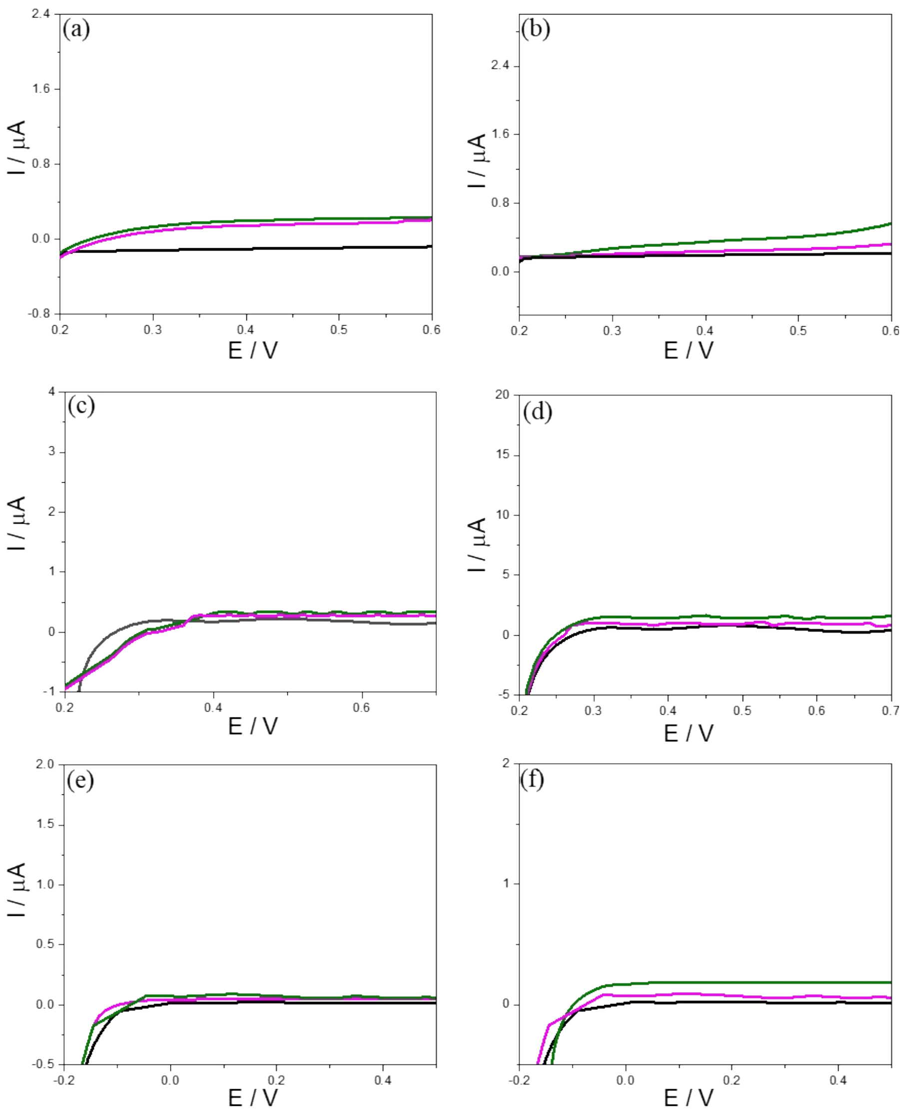



**Fig. S7** Linear sweep voltammetry (LSV) signals of only chiral cages (black line) $[(Me_2CO)(H_2O)@Ni_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (a), $[(Me_2CO)(H_2O)@Ni_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (b), $[(Me_2CO)@Cu_3(s,r\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ (c), $[(Me_2CO)@Cu_3(r,s\text{-}L)_2(H_2O)_9](ClO_4)_6\cdot 7Me_2CO$ (d), $[(Me_2CO)(H_2O)@Zn_3(s,r\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (e), and $[(Me_2CO)(H_2O)@Zn_3(r,s\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (f). Pink line indicates only (*S*)-2-BuOH signal, and green line indicates only (*R*)-2-BuOH signal.

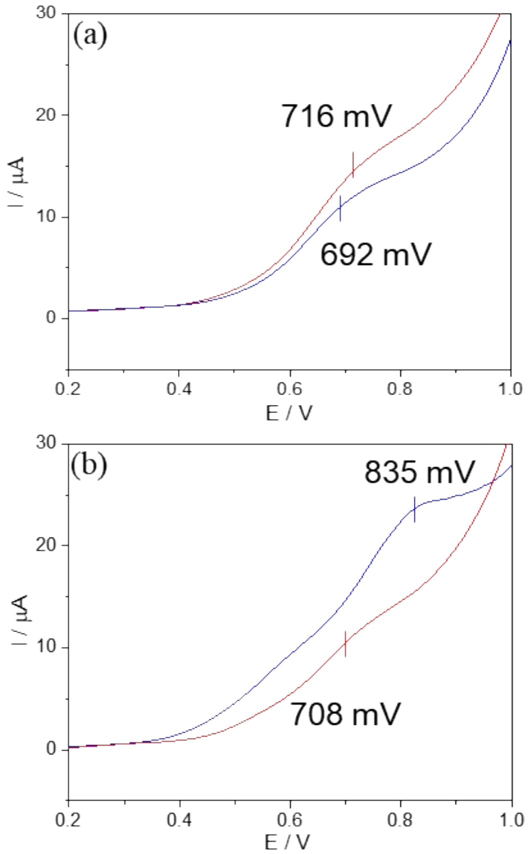



**Fig. S8** Linear sweep voltammetry (LSV) signals of $[(Me_2CO)(H_2O)@Zn_3(\mathit{s,r}\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (a), and $[(Me_2CO)(H_2O)@Zn_3(\mathit{r,s}\text{-}L)_2(H_2O)_{11}](ClO_4)_6\cdot 7Me_2CO$ (b) in presence of 1.0 mM (*S*)-2-BuOH (blue line) and (*R*)-2-BuOH (red line).