<Electronic Supplementary Information>

Pair of chiral molecular ladders and successive hydration in single-crystal-to-single-crystal mode

Junmyeong Park,[a] Dongwon Kim,[a] Dongwook Kim,[b] and Ok-Sang Jung*[a]

[a]Department of Chemistry, Pusan National University, Busan 46241, Republic of Korea Fax: (+82) 51-5163522; Tel: (+82) 51-5103240; E-mail: oksjung@pusan.ac.kr

[b]Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 34141, Republic of Korea

Electronic Supplementary Information (ESI) available: ^{1}H NMR spectra and IR spectra of 1*S*,2*R*-L , 1*R*,2*S*-L , CH_2Cl_2·2CH_3CN@[$Zn_3(NO_3)_6$(1*S*,2*R*-L)$_2$] CH_2Cl_2·2CH_3CN@[$Zn_3(NO_3)_6$(1*R*,2*S*-L)$_2$], 2CH_3CN@[$Zn_3(NO_3)_6$(1*S*,2*R*-L)$_2(H_2O)_2$] and 2CH_3CN@[$Zn_3(NO_3)_6$(1*R*,2*S*-L)$_2(H_2O)_2$]. Crystal structures of, CH_2Cl_2·2CH_3CN@[$Zn_3(NO_3)_6$(1*S*,2*R*-L)$_2$] CH_2Cl_2·2CH_3CN@[$Zn_3(NO_3)_6$(1*R*,2*S*-L)$_2$], 2CH_3CN@[$Zn_3(NO_3)_6$(1*S*,2*R*-L)$_2(H_2O)_2$] and 2CH_3CN@[$Zn_3(NO_3)_6$(1*R*,2*S*-L)$_2(H_2O)_2$]. PXRD patterns of CH_2Cl_2·2CH_3CN@[$Zn_3(NO_3)_6$(1*S*,2*R*-L)$_2$], CH_2Cl_2·2CH_3CN@[$Zn_3(NO_3)_6$(1*R*,2*S*-L)$_2$], 2CH_3CN@[$Zn_3(NO_3)_6$(1*S*,2*R*-L)$_2(H_2O)_2$] and 2CH_3CN@[$Zn_3(NO_3)_6$(1*R*,2*S*-L)$_2(H_2O)_2$].

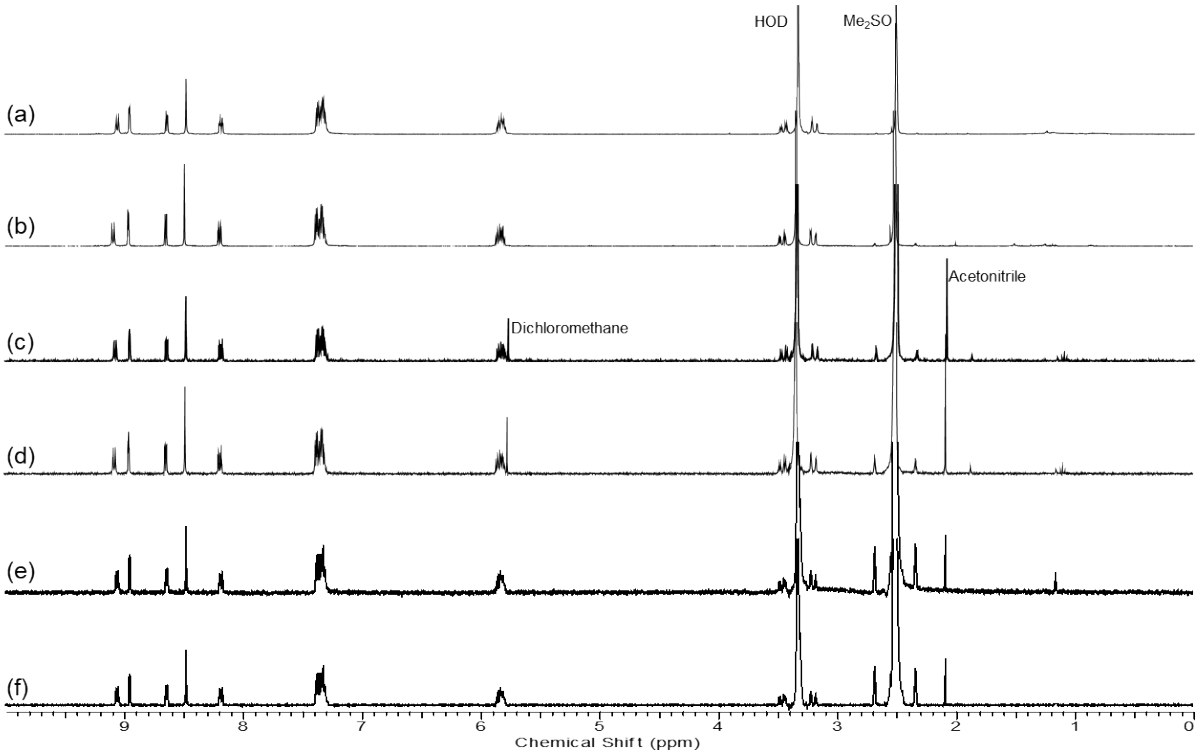


Fig. S1 ^{1}H NMR spectra for 1*S*,2*R*-L (a), 1*R*,2*S*-L (b). $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2]$ (c), $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2]$ (d), $2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2(H_2O)_2]$ (e), $2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2(H_2O)_2]$ (f).

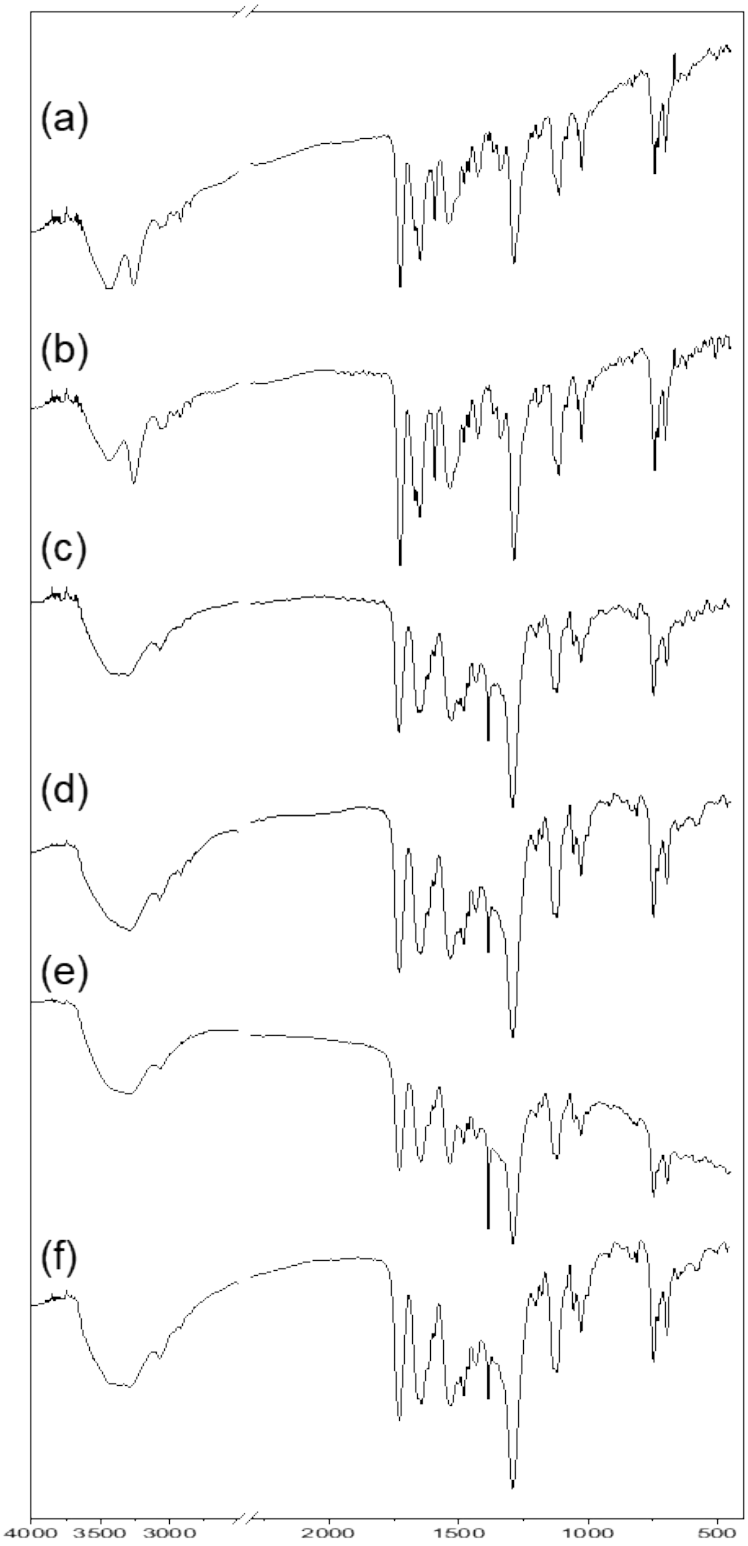


Fig. S2 IR spectra for 1*S*,2*R*-L (a), 1*R*,2*S*-L (b). $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2]$ (c), $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2]$ (d), $2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2(H_2O)_2]$ (e), $2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2(H_2O)_2]$ (f).

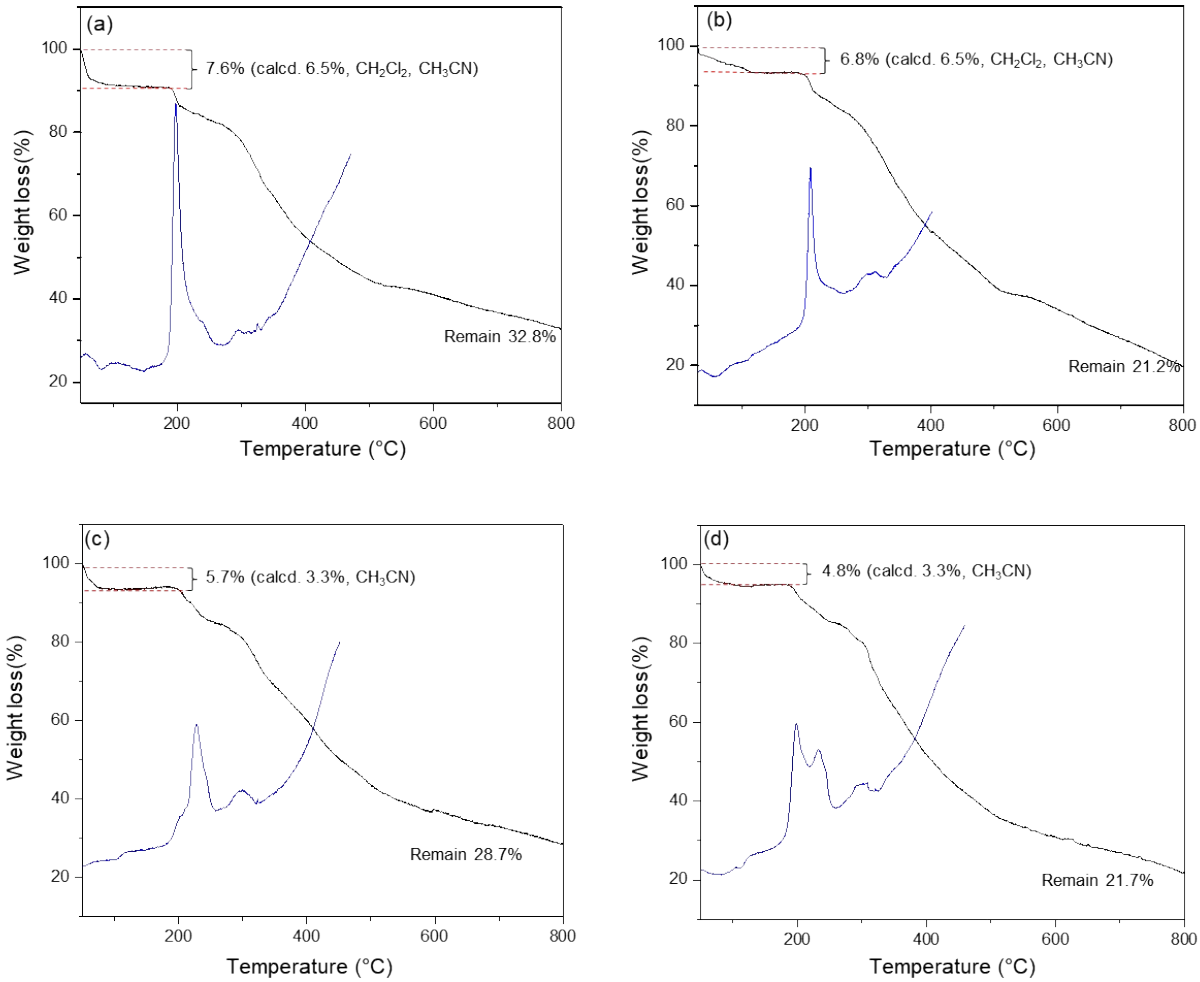


Fig. S3 TG and DSC curves for $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-L})_2]$ (a), $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-L})_2]$ (b), $2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-L})_2(H_2O)_2]$ (c), $2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-L})_2(H_2O)_2]$ (d).

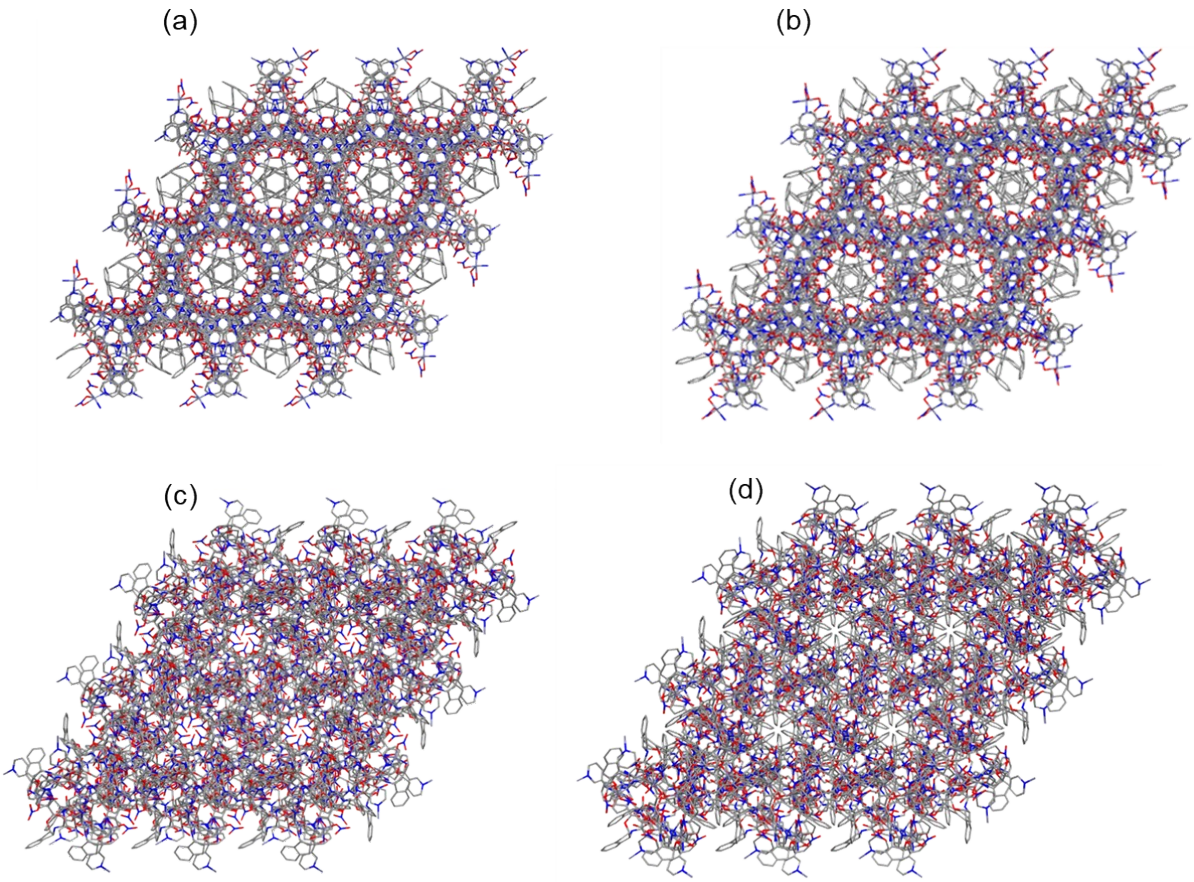


Fig. S4 Packing structure of $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2]$ (a), $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2]$ (b), $2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2(H_2O)_2]$ (c), and $2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2(H_2O)_2]$ (d).

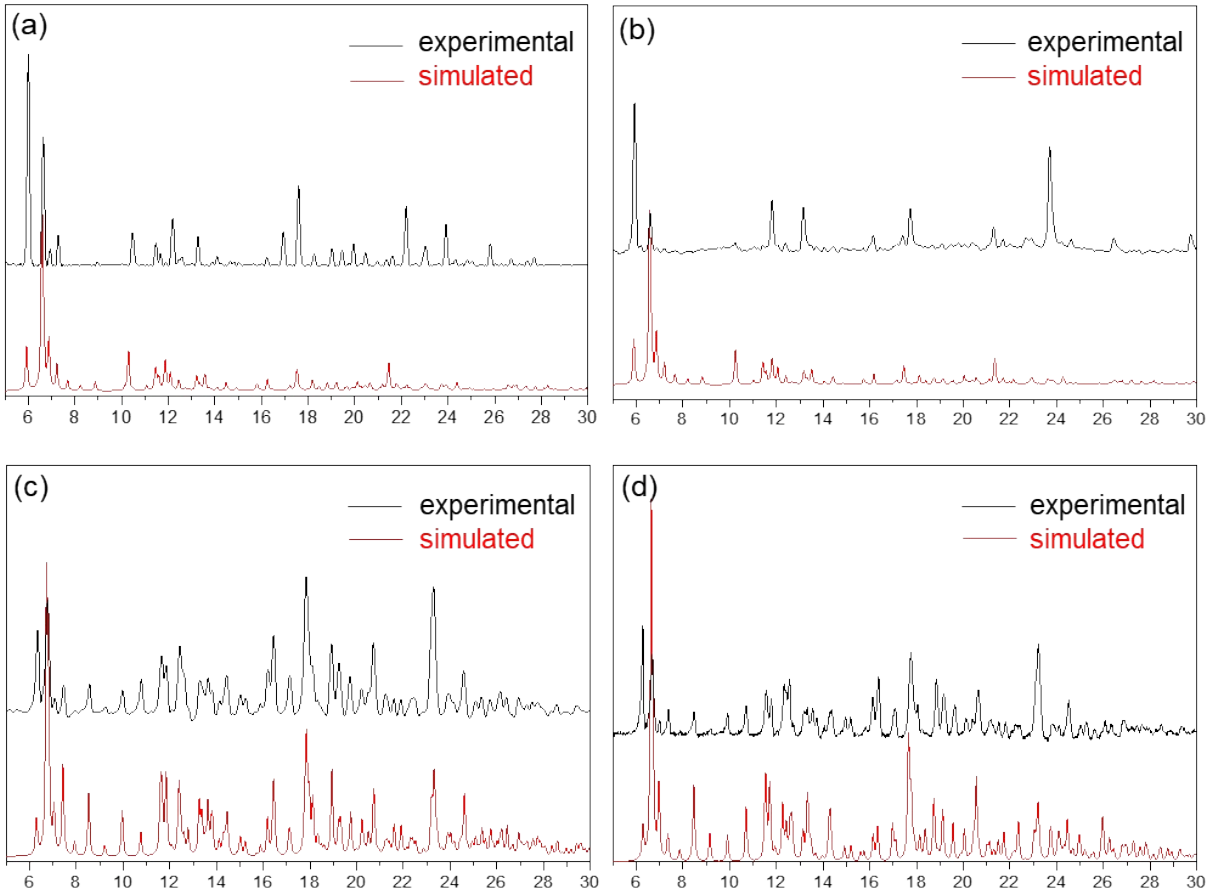


Fig. S5 PXRD patterns of $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2]$ (a), $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2]$ (b), $2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2(H_2O)_2]$ (c), $2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2(H_2O)_2]$ (d).

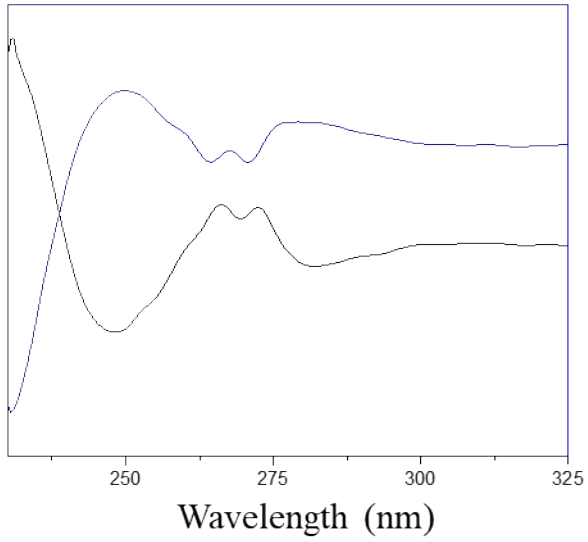
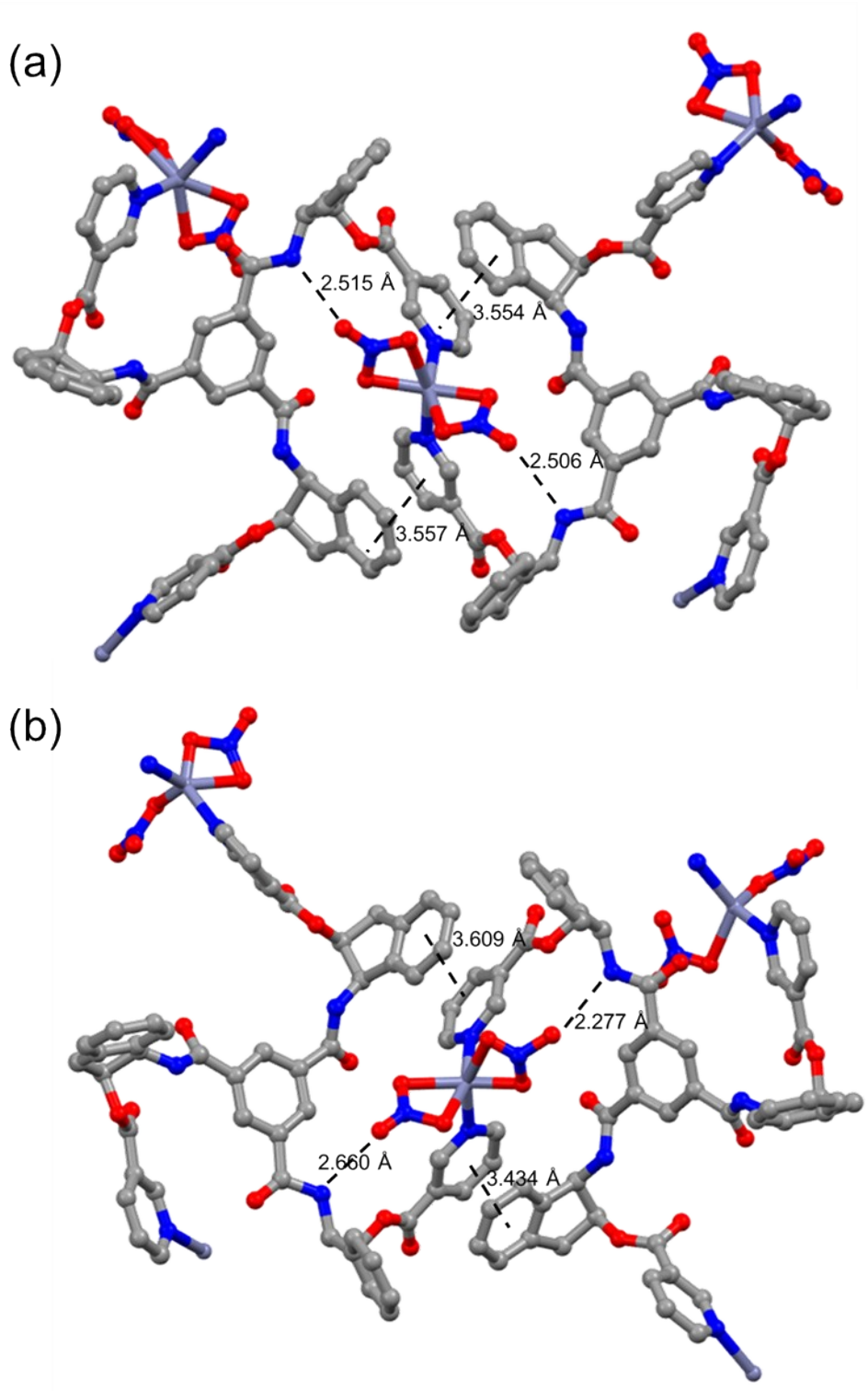


Fig. S6. Circular dichroism (CD) spectra of 1*R*,2*S*-L (blue line) and 1*S*,2*R*-L (black line).


(a)
2.515 Å
3.554 Å
2.506 Å
3.557 Å
(b)
3.609 Å
2.277 Å
2.660 Å
3.434 Å

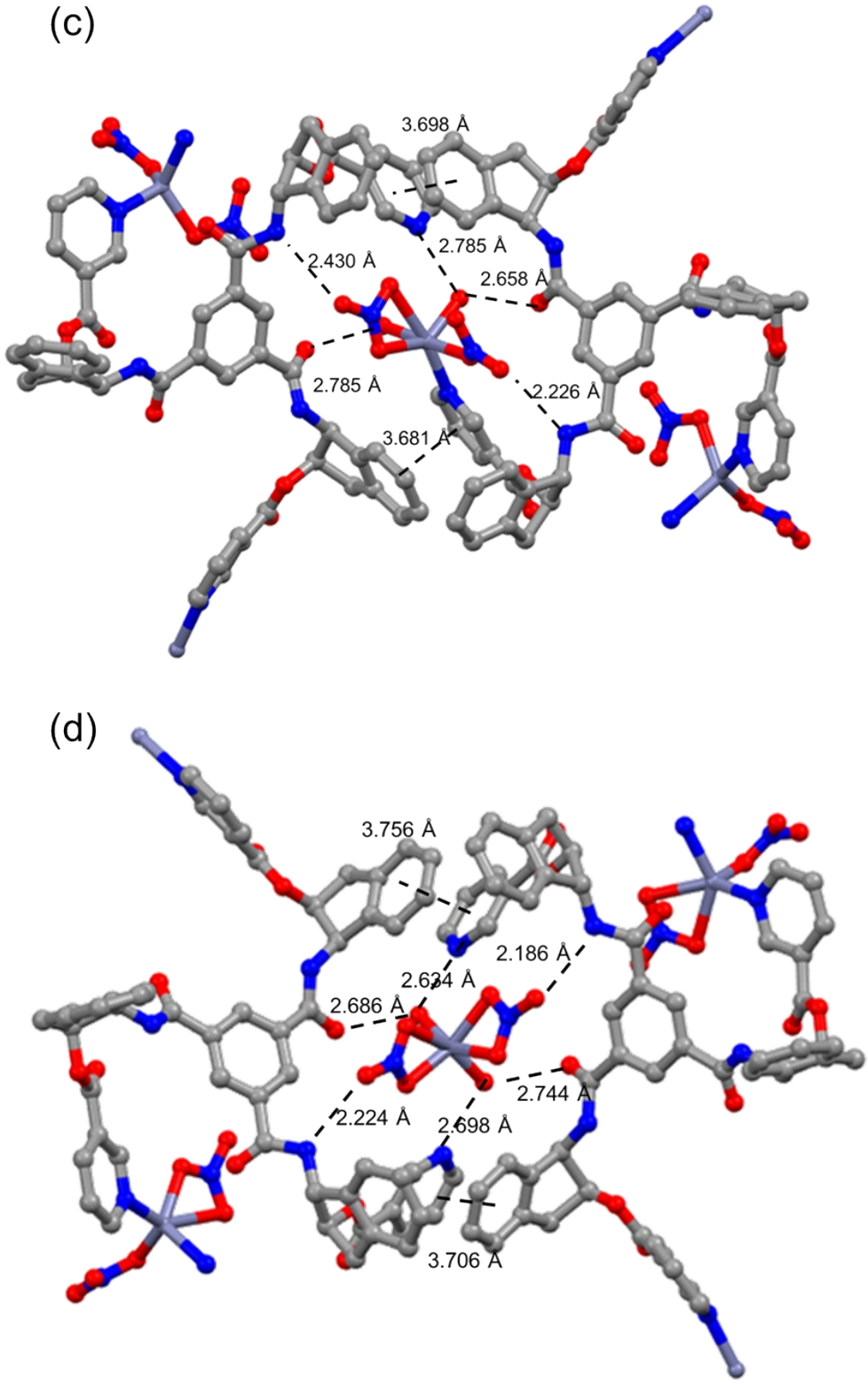


Fig. S7. intermolecular hydrogen bond length of $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2]$ (a), $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2]$ (b), $2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-}L)_2(H_2O)_2]$ (c), $2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-}L)_2(H_2O)_2]$ (d). (H atoms are omitted for clarity)

Table S1. Selected bond lengths and angles for $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-L})_2]$ (a), $CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-L})_2]$ (b), $2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-L})_2(H_2O)_2]$ (c), $2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-L})_2(H_2O)_2]$ (d)

$CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6((1S,2R)\text{-L})_2]$	$CH_2Cl_2 \cdot 2CH_3CN@[Zn_3(NO_3)_6((1R,2S)\text{-L})_2]$	$2CH_3CN@[Zn_3(NO_3)_6(1S,2R\text{-L})_2(H_2O)_2]$	$2CH_3CN@[Zn_3(NO_3)_6(1R,2S\text{-L})_2(H_2O)_2]$
Zn(1)-O(20)	Zn(1)-N(28A)	Zn(1)-O(16)	Zn(1A)-N(23A)
Zn(1)-N(2)	Zn(1)-O(17)	Zn(1)-O(12)	Zn(1A)-O(77A)
Zn(1)-N(8)$^{\#1}$	Zn(1)-O(17D)	Zn(1)-O(16D)	Zn(1A)-O(72A)
Zn(1)-O(19)	Zn(1)-O(16D)	Zn(1)-N(28A)	Zn(1A)-N(65A)$^{\#1}$
Zn(1)-N(14)	Zn(1)-O(12)	Zn(1)-N(70A)$^{\#1}$	Zn(1B)-N(23B)
Zn(2)-N(4)$^{\#2}$	Zn(1)-N(70A)$^{\#1}$	Zn(1)-O(16E)	Zn(1B)-N(44B)$^{\#2}$
Zn(2)-O(03X)	Zn(1)-O(12D)	Zn(2)-O(29)	Zn(1B)-O(77B)
Zn(2)-O(78)	Zn(1)-C(27A)	Zn(2)-O(22D)	Zn(1B)-O(72B)
Zn(2)-N(6)	Zn(2)-O(22)	Zn(2)-O(22)	Zn(1B)-O(74B)
Zn(2)-O(79)	Zn(2)-N(49A)	Zn(2)-O(26)	Zn(1C)-O(12C)
Zn(3)-O(28)	Zn(2)-N(28B)	Zn(2)-N(28B)	Zn(1C)-O(11C)
Zn(3)-N(10)	Zn(2)-O(28)	Zn(2)-O(30)	Zn(1C)-O(3C)
Zn(3)-N(19)$^{\#3}$	Zn(2)-O(26)	Zn(2)-O(27)	Zn(1C)-O(7C)
Zn(3)-O(25)	Zn(2)-O(23)	Zn(3)-O(32D)	Zn(1C)-O(9C)
Zn(3)-O(26)	Zn(3)-O(32)	Zn(3)-N(49B)	Zn(1C)-O(5C)
	Zn(3)-O(33)	Zn(3)-O(36)	
O(20)-Zn(1)-N(2)	Zn(3)-N(49B)	Zn(3)-O(32)	N(23A)-Zn(1A)-O(77A)
O(20)-Zn(1)-N(8)$^{\#1}$	Zn(3)-O(36D)	Zn(3)-O(36D)	N(23A)-Zn(1A)-O(72A)
N(2)-Zn(1)-N(8)$^{\#1}$	Zn(3)-N(31)	Zn(3)-N(70B)$^{\#2}$	O(77A)-Zn(1A)-O(72A)
O(20)-Zn(1)-O(22)	Zn(3)-O(32D)		N(23A)-Zn(1A)-(65A)$^{\#1}$
N(2)-Zn(1)-O(22)	Zn(3)-O(36)	O(16)-Zn(1)-O(12)	O(77A)-Zn(1A)N(65A)$^{\#1}$
N(8)$^{\#1}$-Zn(1)-O(22)	Zn(3)-N(70B)$^{\#1}$	O(12)-Zn(1)-O(16D)	O(72A)-Zn(1A)-(65A)$^{\#1}$
O(20)-Zn(1)-O(19)		O(16)-Zn(1)-N(28A)	N(23B)-Zn(1B)-N(44B)$^{\#2}$
N(2)-Zn(1)-O(19)	N(28A)-Zn(1)-O(17)	O(12)-Zn(1)-N(28A)	N(23B)-Zn(1B)-O(77B)
N(8)$^{\#1}$-Zn(1)-O(19)	N(28A)-Zn(1)-O(17D)	O(16D)-Zn(1)-N(28A)	N(44B)$^{\#2}$-Zn(1B)-O(77B)
O(22)-Zn(1)-O(19)	N(28A)-Zn(1)-O(16D)	O(16)-Zn(1)-N(70A)$^{\#1}$	N(23B)-Zn(1B)-O(72B)
O(20)-Zn(1)-O(23)	O(17D)-Zn(1)-O(16D)	O(12)-Zn(1)-N(70A)$^{\#1}$	N(44B)$^{\#2}$-Zn(1B)-O(72B)
N(2)-Zn(1)-O(23)	N(28A)-Zn(1)-O(12)	N(28A)-Zn(1)-N(70A)$^{\#1}$	O(77B)-Zn(1B)-O(72B)
N(8)$^{\#1}$-Zn(1)-O(23)	O(17)-Zn(1)-O(12)	O(12)-Zn(1)-O(16E)	N(23B)-Zn(1B)-O(74B)
O(22)-Zn(1)-O(23)	N(28A)-Zn(1)-N(70A)$^{\#1}$	N(28A)-Zn(1)-O(16E)	N(44B)$^{\#2}$-Zn(1B)-O(74B)
O(19)-Zn(1)-O(23)	O(17)-Zn(1)-N(70A)$^{\#1}$	N(70A)$^{\#1}$-Zn(1)-O(16E)	O(77B)-Zn(1B)-O(74B)
O(20)-Zn(1)-N(14)	O(12)-Zn(1)-N(70A)$^{\#1}$	O(29)-Zn(2)-O(22D)	O(72B)-Zn(1B)-O(74B)
N(2)-Zn(1)-N(14)	N(28A)-Zn(1)-O(12D)	O(29)-Zn(2)-O(22)	O(12C)-Zn(1C)-O(11C)
N(8)$^{\#1}$-Zn(1)-N(14)	O(17D)-Zn(1)-O(12D)	O(29)-Zn(2)-O(26)	O(12C)-Zn(1C)-O(3C)
O(22)-Zn(1)-N(14)	O(16D)-Zn(1)-O(12D)	O(22D)-Zn(2)-O(26)	O(11C)-Zn(1C)-O(3C)
O(19)-Zn(1)-N(14)	N(70A)$^{\#1}$-Zn(1)-O(12D)	O(22)-Zn(2)-O(26)	O(12C)-Zn(1C)-O(7C)
O(23)-Zn(1)-N(14)	N(28A)-Zn(1)-C(27A)	O(29)-Zn(2)-N(28B)	O(11C)-Zn(1C)-O(7C)
N(4)$^{\#2}$-Zn(2)-O(03X)	O(17)-Zn(1)-C(27A)	O(22D)-Zn(2)-N(28B)	O(3C)-Zn(1C)-O(7C)
N(4)$^{\#2}$-Zn(2)-O(78)	O(17D)-Zn(1)-C(27A)	O(22)-Zn(2)-N(28B)	O(12C)-Zn(1C)-O(9C)
O(03X)-Zn(2)-O(78)	O(16D)-Zn(1)-C(27A)	O(26)-Zn(2)-N(28B)	O(11C)-Zn(1C)-O(9C)
N(4)$^{\#2}$-Zn(2)-N(6)	O(12)-Zn(1)-C(27A)	O(29)-Zn(2)-O(30)	O(3C)-Zn(1C)-O(9C)
O(03X)-Zn(2)-N(6)	N(70A)$^{\#1}$-Zn(1)-C(27A)	O(22D)-Zn(2)-O(30)	O(7C)-Zn(1C)-O(9C)
O(78)-Zn(2)-N(6)	O(12D)-Zn(1)-C(27A)	O(22)-Zn(2)-O(30)	O(12C)-Zn(1C)-O(5C)
N(4)$^{\#2}$-Zn(2)-O(79)	O(22)-Zn(2)-N(49A)	O(26)-Zn(2)-O(30)	O(11C)-Zn(1C)-O(5C)
O(03X)-Zn(2)-O(79)	O(22)-Zn(2)-N(28B)	N(28B)-Zn(2)-O(30)	O(3C)-Zn(1C)-O(5C)
O(78)-Zn(2)-O(79)	N(49A)-Zn(2)-N(28B)	O(29)-Zn(2)-O(27)	O(7C)-Zn(1C)-O(5C)
N(6)-Zn(2)-O(79)	O(22)-Zn(2)-O(28)	O(22D)-Zn(2)-O(27)	O(9C)-Zn(1C)-O(5C)
O(28)-Zn(3)-N(10)	N(49A)-Zn(2)-O(28)	O(22)-Zn(2)-O(27)	
O(28)-Zn(3)-N(19)$^{\#3}$	N(28B)-Zn(2)-O(28)	O(26)-Zn(2)-O(27)	
N(10)-Zn(3)-N(19)$^{\#3}$	O(22)-Zn(2)-O(26)	N(28B)-Zn(2)-O(27)	

O(28)-Zn(3)-O(25)
N(10)-Zn(3)-O(25)
N(19)#3-Zn(3)-O(25)
O(28)-Zn(3)-O(26)
N(10)-Zn(3)-O(26)
N(19)#3-Zn(3)-O(26)
O(25)-Zn(3)-O(26)

N(49A)-Zn(2)-O(26)
N(28B)-Zn(2)-O(26)
O(28)-Zn(2)-O(26)
O(22)-Zn(2)-O(23)
N(49A)-Zn(2)-O(23)
N(28B)-Zn(2)-O(23)
O(28)-Zn(2)-O(23)
O(26)-Zn(2)-O(23)
O(32)-Zn(3)-O(33)
O(32)-Zn(3)-N(49B)
O(33)-Zn(3)-N(49B)
N(49B)-Zn(3)-O(36D)
O(32)-Zn(3)-N(31)
O(33)-Zn(3)-N(31)
N(49B)-Zn(3)-N(31)
N(49B)-Zn(3)-O(32D)
O(36D)-Zn(3)-O(32D)
O(32)-Zn(3)-O(36)
O(33)-Zn(3)-O(36)
N(49B)-Zn(3)-O(36)
N(31)-Zn(3)-O(36)
O(32)-Zn(3)-N(70B)#1
O(33)-Zn(3)-N(70B)#1
N(49B)-Zn(3)-(70B)#1
O(36D)-Zn(3)-(70B)#1
N(31)-Zn(3)-N(70B)#1
O(32D)-Zn(3)-(70B)#1
O(36)-Zn(3)-N(70B)#1

O(30)-Zn(2)-O(27)
O(32D)-Zn(3)-N(49B)
N(49B)-Zn(3)-O(36)
N(49B)-Zn(3)-O(32)
O(36)-Zn(3)-O(32)
O(32D)-Zn(3)-O(36D)
N(49B)-Zn(3)-O(36D)
O(32D)-Zn(3)-N(70B)#2
N(49B)-Zn(3)-N(70B)#2
O(36)-Zn(3)-N(70B)#2
O(32)-Zn(3)-N(70B)#2
O(36D)-Zn(3)-N(70B)#2

#1 x-y+1,x,z+1/6
#2 x-1,y-1,z
#3 x-1,y,z

#1 x-1,y,z
#2 x+1,y,z

#1 x,y-1,z
#2 x,y+1,z

#1 x+1,y,z
#2 x,y-1,z
#3 x-1,y,z