<Electronic Supplementary Information>

Stepwise coordination isomerism. Adsorption and recognition of CH_2I_2 into 2D layered crystals in SCSC mode

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Electronic Supplementary Information (ESI) available: Experimental details and crystal structure determination. IR spectra of each sample (L, $3CH_2Cl_2{\cdot}2C_2H_5OH$@$[CdI_2L]$, $4C_4H_8O$@$[CdI_2L]$, $3CH_2I_2$@$[CdI_2L]$ and $3CH_2Br_2$@$[CdI_2L]$). TGA/DSC curves of the present Cd(II) compounds, ($3CH_2Cl_2{\cdot}2C_2H_5OH$@$[CdI_2L]$ and $4C_4H_8O$@$[CdI_2L]$). Full ^1H NMR spectra of each sample (L, $3CH_2Cl_2{\cdot}2C_2H_5OH$@$[CdI_2L]$, $4C_4H_8O$@$[CdI_2L]$, $1.3CH_2Cl_2{\cdot}0.8C_2H_5OH{\cdot}1.5CH_2I_2$@$[CdI_2L]$, $0.8\ CH_2Cl_2{\cdot}0.6C_2H_5OH{\cdot}2.5CH_2Br_2$@$[CdI_2L]$, $3CH_2I_2$@$[CdI_2L]$, $3CH_2Br_2$@$[CdI_2L]$ and $3CH_2Cl_2$@$[CdI_2L]$). This material is available free of charge at http://pubs.acs.org. CCDC 2077166 - 2077169 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

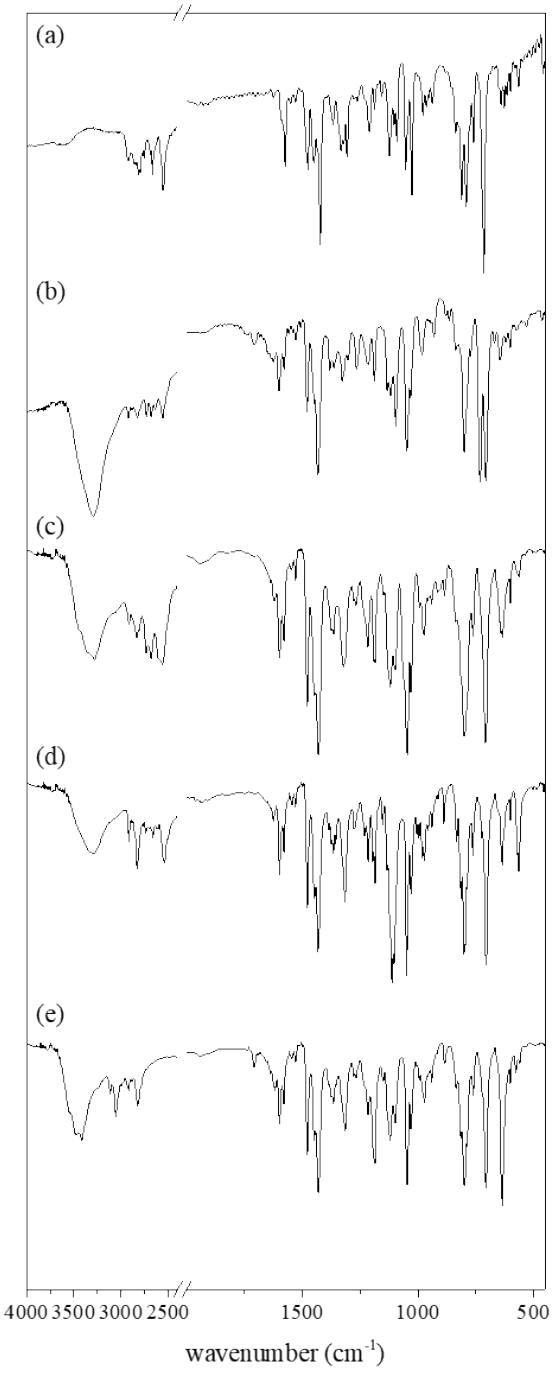

Fig. S1 IR spectra of L (a), $3CH_2Cl_2 \cdot 2C_2H_5OH$@[$CdI_2L$] (b), $4C_4H_8O$@[CdI_2L] (c), $3CH_2I_2$@[CdI_2L] (d), and $3CH_2Br_2$@[CdI_2L] (e).

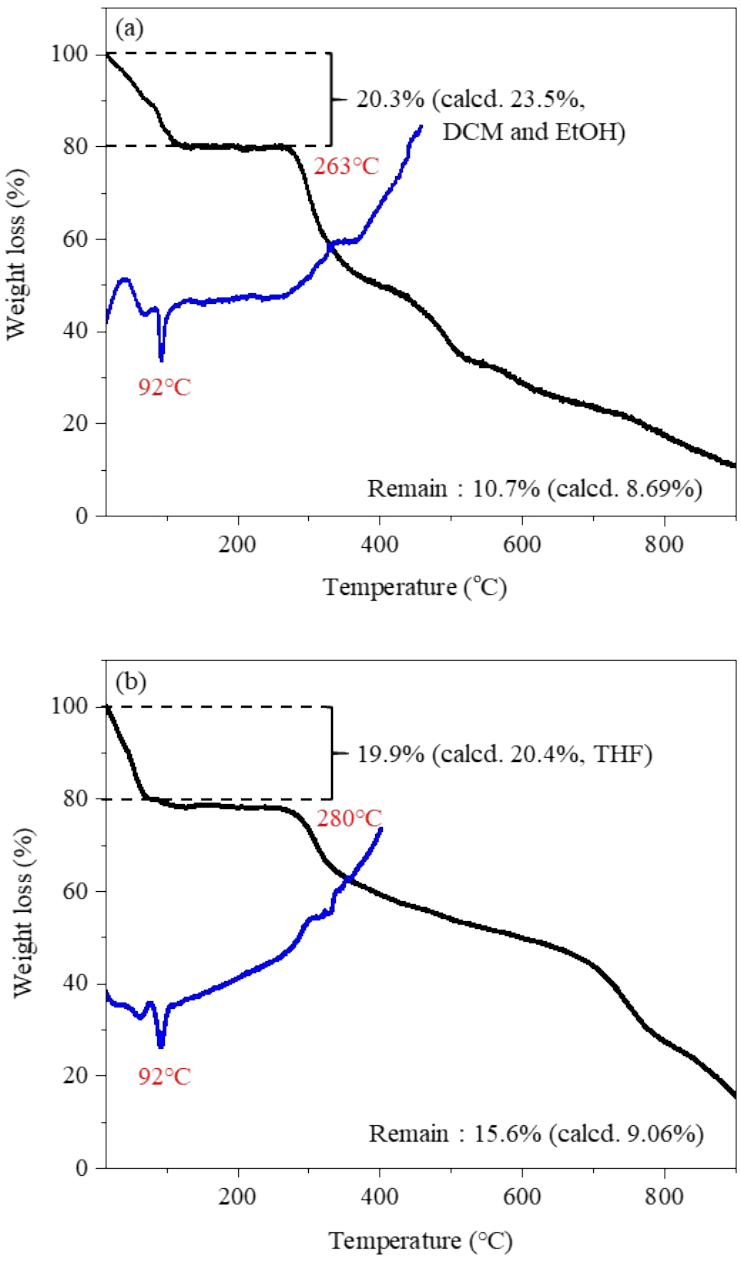

Fig. S2 TGA and DSC overlays of $3CH_2Cl_2 \cdot 2C_2H_5OH$@[$CdI_2L$] (a) and $4C_4H_8O$@[CdI_2L] (b).

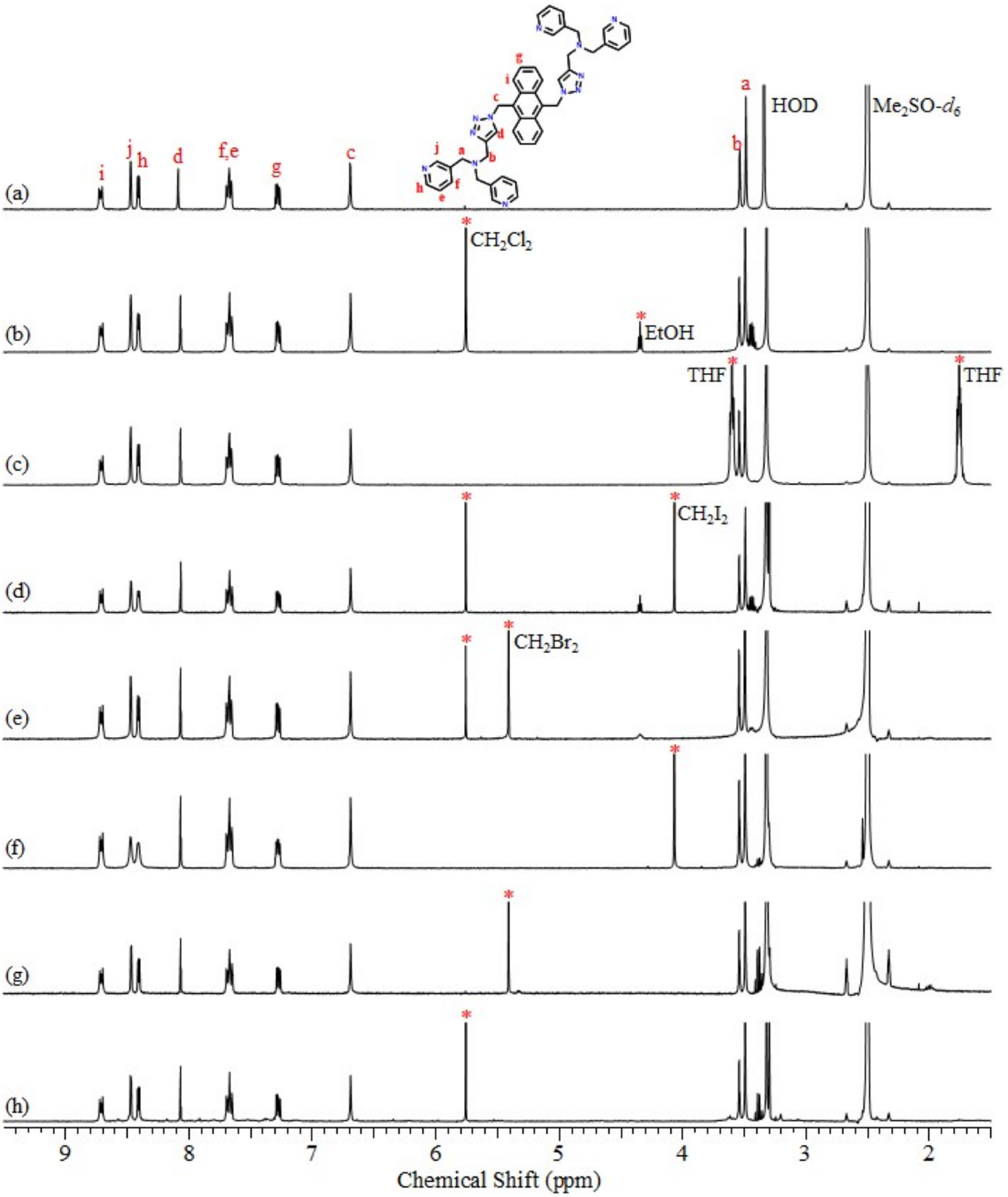

Fig. S3 ^{1}H NMR spectra of L (a), $3CH_2Cl_2{\cdot}2C_2H_5OH@[CdI_2L]$ (b), $4C_4H_8O@[CdI_2L]$ (c), $1.3CH_2Cl_2{\cdot}0.8C_2H_5OH{\cdot}1.5CH_2I_2@[CdI_2L]$ (d), $0.8\ CH_2Cl_2{\cdot}0.6C_2H_5OH{\cdot}2.5CH_2Br_2@[CdI_2L]$ (e), $3CH_2I_2@[CdI_2L]$ (f), $3CH_2Br_2@[CdI_2L]$ (g), and $3CH_2Cl_2@[CdI_2L]$ (h) in Me_2SO-d_6. For spectra (d) and (e), solvate molecules were exchanged from $CH_2Cl_2{\cdot}2C_2H_5OH@[CdI_2L]$. For spectra (f), (g), and (h), guestes were exchanged from $4C_4H_8O@[CdI_2L]$. After the solvate exchange, the crystals were washed with diethyl ether to wash off the solvents on the surface.

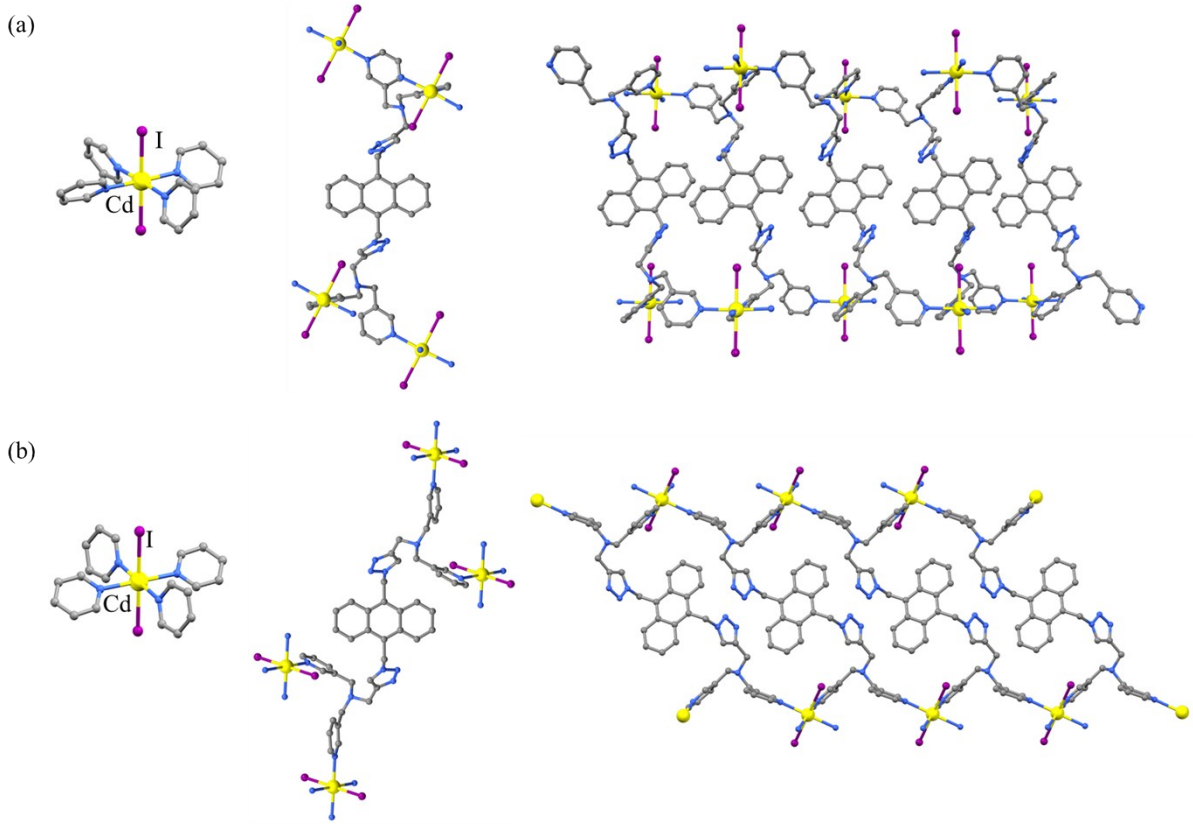

Fig. S4 Detailed crystal structure for $3CH_2Cl_2 \cdot 2C_2H_5OH@[CdI_2L]$ (a) and $4C_4H_8O@[CdI_2L]$ (b) showing octahedral geometry around Cd(II) and conformation around ligands.

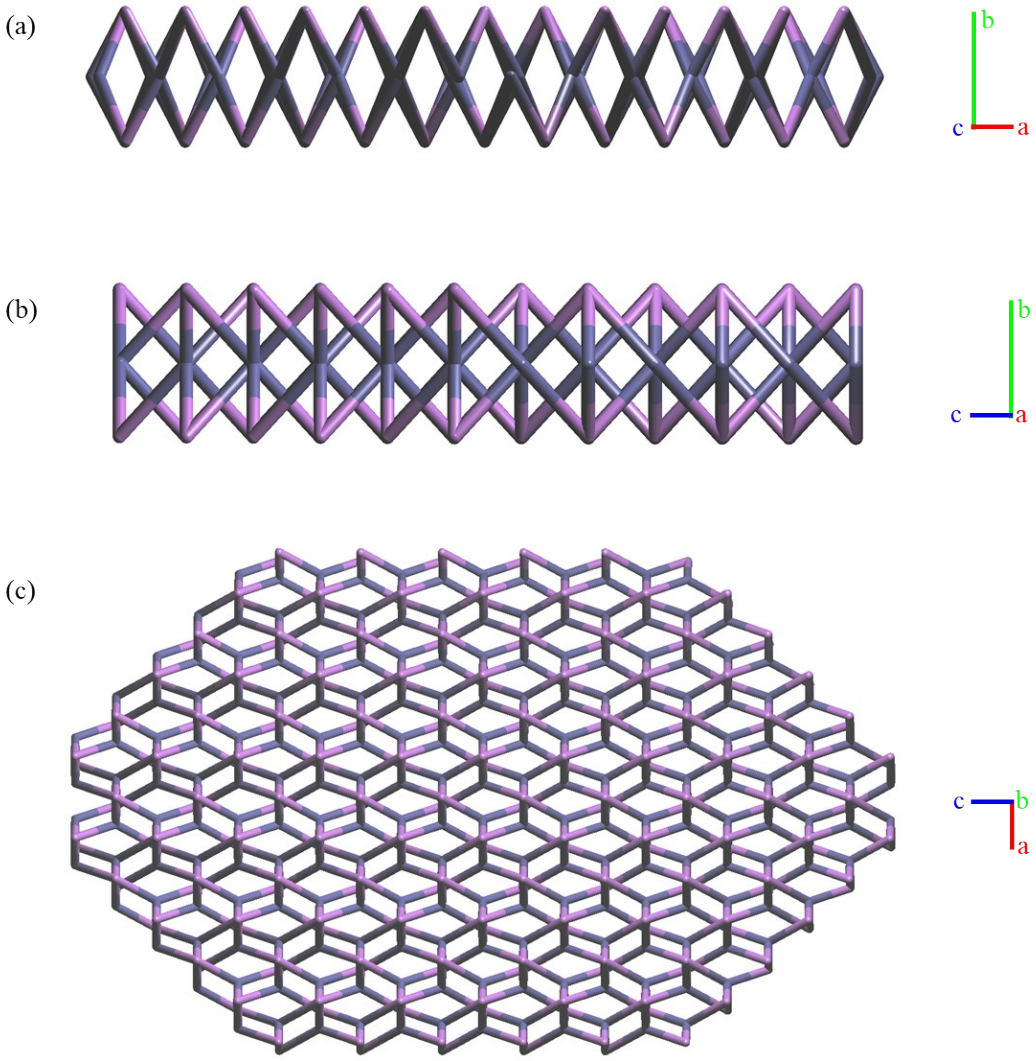

Fig. S5 Topology(new, $\{4^3 \cdot 6^2 \cdot 8\}$) analysis of $3CH_2Cl_2 \cdot 2C_2H_5OH$@$[CdI_2L]$: (a) along c axis, (b) along a axis, and (c) along b axis