

SUPPLEMENTARY MATERIALS

S1. Crystallography

Computing details

Data collection: Bruker *APEX* 2; cell refinement: Bruker *SAINT*; data reduction: Bruker *SAINT*; program(s) used to solve structure: *SIR2004*; program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: Bruker *SHELXTL*; software used to prepare material for publication: Bruker *SHELXTL*.

References

- 1 M. C. Burla, R. Caliendo, M. Camalli, B. Carrozzini, G. L. Casciaro, L. D. Caro, C. Giacovazzo, G. Polidori, and R. Spagna, *J. Appl. Cryst.*, 2005, **38**, 381.
- 2 G.M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112.

(cdzno)

Crystal data

$C_{28}H_{38}Cd_3F_{12}O_{16}$	$Z = 1$
$M_r = 1195.78$	$F(000) = 586$
Triclinic, $P\bar{1}$	$D_x = 1.972 \text{ Mg m}^{-3}$
$a = 9.5553 (4) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 9.6390 (5) \text{ \AA}$	Cell parameters from 7666 reflections
$c = 12.4046 (6) \text{ \AA}$	$\theta = 2.3\text{--}28.3^\circ$
$\alpha = 69.482 (1)^\circ$	$\mu = 1.69 \text{ mm}^{-1}$
$\beta = 70.698 (1)^\circ$	$T = 150 \text{ K}$
$\gamma = 87.293 (1)^\circ$	Block, colourless
$V = 1006.83 (8) \text{ \AA}^3$	$0.47 \times 0.21 \times 0.20 \text{ mm}$

Data collection

Bruker APEX 2 CCD diffractometer	5001 independent reflections
Radiation source: fine-focus sealed tube	4489 reflections with $I > 2\sigma(I)$
Graphite	$R_{\text{int}} = 0.018$
ω rotation with narrow frames scans	$\theta_{\text{max}} = 28.3^\circ$, $\theta_{\text{min}} = 1.9^\circ$
Absorption correction: multi-scan SADABS v2009/1, Sheldrick, G.M., (2009)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.504$, $T_{\text{max}} = 0.729$	$k = -12 \rightarrow 12$
13937 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.027$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.070$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 1.2565P]$ where $P = (F_o^2 + 2F_c^2)/3$
5001 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
268 parameters	$\Delta_{\text{max}} = 1.01 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta_{\text{min}} = -0.55 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F , and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>X</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.194424 (19)	0.55482 (2)	0.347057 (16)	0.02262 (6)
Cd2	0.5000	0.5000	0.5000	0.02304 (7)
O11	0.2923 (2)	0.3376 (2)	0.3518 (2)	0.0378 (5)
O12	0.4752 (2)	0.3152 (2)	0.4317 (2)	0.0385 (5)
F11	0.3406 (3)	0.0244 (2)	0.4340 (2)	0.0653 (7)
C11	0.3990 (3)	0.2802 (3)	0.3810 (2)	0.0250 (5)
F12	0.5727 (3)	0.0993 (3)	0.3493 (2)	0.0611 (6)
C12	0.4374 (4)	0.1378 (4)	0.3511 (3)	0.0380 (7)
F13	0.4279 (3)	0.1522 (3)	0.2426 (2)	0.0582 (6)
O21	0.4186 (2)	0.6865 (3)	0.22018 (19)	0.0398 (5)
O22	0.5969 (2)	0.6611 (2)	0.30628 (18)	0.0357 (5)
C21	0.5424 (3)	0.7114 (3)	0.2238 (2)	0.0259 (5)
C22	0.6456 (3)	0.8276 (4)	0.1056 (3)	0.0386 (7)
F21	0.7869 (2)	0.8034 (4)	0.0844 (2)	0.0821 (9)
F22	0.6291 (5)	0.9592 (3)	0.1076 (3)	0.1324 (18)
F23	0.6220 (3)	0.8273 (4)	0.0066 (2)	0.0868 (10)
O31	0.2676 (2)	0.5675 (2)	0.50198 (16)	0.0266 (4)
O32	0.0273 (2)	0.5821 (3)	0.56922 (19)	0.0363 (5)
C31	0.1501 (3)	0.5819 (3)	0.5834 (2)	0.0246 (5)
C32	0.1637 (3)	0.6036 (4)	0.6935 (3)	0.0381 (7)
H32A	0.2680	0.6004	0.6893	0.057*
H32B	0.1031	0.5243	0.7676	0.057*
H32C	0.1288	0.7001	0.6957	0.057*
O41	0.0916 (2)	0.7792 (2)	0.29939 (18)	0.0294 (4)
C41	0.1669 (4)	0.9080 (4)	0.2963 (4)	0.0536 (9)
H41A	0.2552	0.9446	0.2214	0.064*
H41B	0.1995	0.8830	0.3684	0.064*
C42	0.0563 (6)	1.0226 (6)	0.2976 (7)	0.0895 (19)
H42A	0.0265	1.0403	0.3758	0.107*
H42B	0.0991	1.1176	0.2298	0.107*
C43	-0.0727 (5)	0.9635 (5)	0.2827 (6)	0.0892 (19)
H43A	-0.0664	1.0018	0.1959	0.107*
H43B	-0.1666	0.9916	0.3318	0.107*
C44	-0.0656 (3)	0.7998 (4)	0.3270 (3)	0.0449 (8)
H44A	-0.1194	0.7553	0.4160	0.054*
H44B	-0.1092	0.7543	0.2840	0.054*

O51	0.1849 (2)	0.5739 (2)	0.15308 (17)	0.0312 (4)
C51	0.2702 (5)	0.4818 (5)	0.0907 (3)	0.0591 (11)
H51A	0.2294	0.3770	0.1339	0.071*
H51B	0.3751	0.4879	0.0867	0.071*
C52	0.2605 (7)	0.5380 (6)	-0.0346 (4)	0.0770 (16)
H52A	0.2013	0.4651	-0.0451	0.092*
H52B	0.3610	0.5556	-0.0968	0.092*
C53	0.1863 (5)	0.6803 (5)	-0.0476 (3)	0.0597 (11)
H53A	0.2438	0.7607	-0.1239	0.072*
H53B	0.0842	0.6682	-0.0480	0.072*
C54	0.1837 (6)	0.7131 (4)	0.0613 (3)	0.0659 (13)
H54A	0.2719	0.7792	0.0415	0.079*
H54B	0.0930	0.7626	0.0899	0.079*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01808 (9)	0.03211 (11)	0.02080 (9)	0.00271 (7)	-0.00982 (7)	-0.01008 (7)
Cd2	0.02101 (12)	0.02993 (14)	0.02256 (13)	0.00238 (9)	-0.01126 (10)	-0.01081 (10)
O11	0.0387 (11)	0.0434 (12)	0.0471 (13)	0.0151 (9)	-0.0256 (10)	-0.0254 (10)
O12	0.0368 (11)	0.0424 (12)	0.0567 (14)	0.0102 (9)	-0.0278 (10)	-0.0312 (11)
F11	0.093 (2)	0.0325 (11)	0.0775 (17)	-0.0095 (12)	-0.0413 (15)	-0.0140 (11)
C11	0.0247 (12)	0.0270 (12)	0.0241 (12)	0.0010 (10)	-0.0080 (10)	-0.0102 (10)
F12	0.0613 (14)	0.0653 (14)	0.0910 (17)	0.0387 (11)	-0.0464 (13)	-0.0528 (13)
C12	0.0469 (17)	0.0364 (16)	0.0442 (17)	0.0109 (13)	-0.0258 (14)	-0.0213 (14)
F13	0.0815 (16)	0.0647 (14)	0.0590 (13)	0.0275 (12)	-0.0418 (12)	-0.0438 (12)
O21	0.0246 (10)	0.0608 (14)	0.0280 (10)	-0.0083 (9)	-0.0086 (8)	-0.0074 (10)
O22	0.0285 (10)	0.0441 (12)	0.0298 (10)	-0.0004 (9)	-0.0124 (8)	-0.0045 (9)
C21	0.0226 (12)	0.0267 (12)	0.0254 (12)	0.0002 (10)	-0.0061 (10)	-0.0074 (10)
C22	0.0326 (15)	0.0394 (16)	0.0319 (15)	-0.0030 (12)	-0.0084 (12)	-0.0004 (12)
F21	0.0285 (11)	0.119 (2)	0.0562 (14)	-0.0091 (12)	-0.0012 (10)	0.0086 (14)
F22	0.171 (4)	0.0308 (13)	0.109 (3)	-0.0228 (18)	0.049 (2)	-0.0098 (15)
F23	0.0688 (16)	0.132 (3)	0.0317 (11)	-0.0330 (16)	-0.0154 (11)	0.0073 (13)
O31	0.0234 (9)	0.0392 (10)	0.0223 (9)	0.0050 (7)	-0.0099 (7)	-0.0151 (8)
O32	0.0231 (9)	0.0490 (12)	0.0328 (10)	-0.0046 (8)	-0.0131 (8)	-0.0053 (9)
C31	0.0232 (12)	0.0274 (12)	0.0238 (12)	0.0002 (9)	-0.0092 (10)	-0.0084 (10)
C32	0.0297 (14)	0.064 (2)	0.0323 (15)	0.0079 (13)	-0.0113 (12)	-0.0300 (15)

O41	0.0256 (9)	0.0318 (10)	0.0322 (10)	0.0024 (7)	-0.0111 (8)	-0.0116 (8)
C41	0.052 (2)	0.0332 (17)	0.082 (3)	0.0008 (15)	-0.030 (2)	-0.0198 (18)
C42	0.076 (3)	0.059 (3)	0.161 (6)	0.026 (2)	-0.046 (4)	-0.068 (4)
C43	0.055 (3)	0.049 (2)	0.140 (5)	0.019 (2)	-0.025 (3)	-0.014 (3)
C44	0.0273 (15)	0.0450 (18)	0.053 (2)	0.0063 (13)	-0.0136 (14)	-0.0071 (15)
O51	0.0361 (10)	0.0372 (11)	0.0228 (9)	0.0036 (8)	-0.0131 (8)	-0.0105 (8)
C51	0.085 (3)	0.068 (3)	0.0388 (18)	0.036 (2)	-0.031 (2)	-0.0308 (18)
C52	0.116 (4)	0.090 (3)	0.038 (2)	0.053 (3)	-0.036 (2)	-0.034 (2)
C53	0.087 (3)	0.066 (3)	0.0326 (17)	0.022 (2)	-0.0305 (19)	-0.0184 (17)
C54	0.126 (4)	0.046 (2)	0.0357 (18)	0.020 (2)	-0.043 (2)	-0.0132 (16)

Geometric parameters (Å, °)

Cd1—O11	2.242 (2)	O21—C21	1.236 (3)
Cd1—O32 ⁱ	2.271 (2)	O22—C21	1.239 (3)
Cd1—O31	2.2926 (17)	C21—C22	1.541 (4)
Cd1—O41	2.2975 (19)	C22—F22	1.278 (4)
Cd1—O21	2.303 (2)	C22—F21	1.314 (4)
Cd1—O51	2.3799 (18)	C22—F23	1.321 (4)
Cd1—O32	2.788 (2)	O31—C31	1.278 (3)
Cd1—Cd2	3.9010 (2)	O32—C31	1.242 (3)
Cd1—Cd1 ⁱ	4.1904 (4)	O32—Cd1 ⁱ	2.2715 (19)
Cd2—O22	2.257 (2)	C31—C32	1.498 (4)
Cd2—O22 ⁱⁱ	2.257 (2)	O41—C44	1.446 (4)
Cd2—O12	2.276 (2)	O41—C41	1.447 (4)
Cd2—O12 ⁱⁱ	2.276 (2)	C41—C42	1.493 (6)
Cd2—O31 ⁱⁱ	2.2793 (18)	C42—C43	1.472 (7)
Cd2—O31	2.2794 (18)	C43—C44	1.484 (6)
O11—C11	1.236 (3)	O51—C54	1.426 (4)
O12—C11	1.230 (3)	O51—C51	1.431 (4)
F11—C12	1.337 (4)	C51—C52	1.490 (5)
C11—C12	1.541 (4)	C52—C53	1.497 (6)
F12—C12	1.323 (4)	C53—C54	1.484 (5)
C12—F13	1.338 (4)		
O11—Cd1—O32 ⁱ	84.54 (8)	F11—C12—F13	106.4 (3)
O11—Cd1—O31	93.94 (7)	F12—C12—C11	113.1 (2)

O32 ⁱ —Cd1—O31	108.50 (7)	F11—C12—C11	110.1 (3)
O11—Cd1—O41	166.64 (7)	F13—C12—C11	111.7 (2)
O32 ⁱ —Cd1—O41	94.43 (7)	C21—O21—Cd1	139.55 (19)
O31—Cd1—O41	99.00 (7)	C21—O22—Cd2	131.37 (18)
O11—Cd1—O21	91.85 (9)	O21—C21—O22	131.3 (3)
O32 ⁱ —Cd1—O21	166.26 (8)	O21—C21—C22	114.1 (2)
O31—Cd1—O21	84.94 (7)	O22—C21—C22	114.5 (2)
O41—Cd1—O21	86.02 (8)	F22—C22—F21	108.3 (3)
O11—Cd1—O51	85.38 (7)	F22—C22—F23	107.0 (3)
O32 ⁱ —Cd1—O51	87.11 (7)	F21—C22—F23	103.5 (3)
O31—Cd1—O51	164.26 (7)	F22—C22—C21	111.5 (3)
O41—Cd1—O51	81.27 (7)	F21—C22—C21	113.1 (3)
O21—Cd1—O51	79.37 (7)	F23—C22—C21	112.9 (3)
O22—Cd2—O22 ⁱⁱ	179.999 (1)	C31—O31—Cd2	134.42 (16)
O22—Cd2—O12	90.84 (8)	C31—O31—Cd1	106.46 (15)
O22 ⁱⁱ —Cd2—O12	89.16 (8)	Cd2—O31—Cd1	117.13 (8)
O22—Cd2—O12 ⁱⁱ	89.16 (8)	C31—O32—Cd1 ⁱ	140.45 (18)
O22 ⁱⁱ —Cd2—O12 ⁱⁱ	90.84 (8)	O32—C31—O31	120.1 (2)
O12—Cd2—O12 ⁱⁱ	180.00 (10)	O32—C31—C32	120.8 (2)
O22—Cd2—O31 ⁱⁱ	89.96 (7)	O31—C31—C32	119.1 (2)
O22 ⁱⁱ —Cd2—O31 ⁱⁱ	90.04 (7)	C44—O41—C41	109.0 (2)
O12—Cd2—O31 ⁱⁱ	89.33 (7)	C44—O41—Cd1	125.77 (18)
O12 ⁱⁱ —Cd2—O31 ⁱⁱ	90.67 (7)	C41—O41—Cd1	118.80 (18)
O22—Cd2—O31	90.04 (7)	O41—C41—C42	106.0 (3)
O22 ⁱⁱ —Cd2—O31	89.96 (7)	C43—C42—C41	106.3 (4)
O12—Cd2—O31	90.67 (7)	C42—C43—C44	105.1 (4)
O12 ⁱⁱ —Cd2—O31	89.33 (7)	O41—C44—C43	104.4 (3)
O31 ⁱⁱ —Cd2—O31	179.998 (1)	C54—O51—C51	106.5 (3)
C11—O11—Cd1	132.24 (18)	C54—O51—Cd1	122.4 (2)
C11—O12—Cd2	139.15 (19)	C51—O51—Cd1	120.12 (18)
O12—C11—O11	131.1 (3)	O51—C51—C52	106.7 (3)
O12—C11—C12	115.9 (2)	C51—C52—C53	106.3 (3)
O11—C11—C12	112.9 (2)	C54—C53—C52	104.0 (3)
F12—C12—F11	107.9 (3)	O51—C54—C53	106.5 (3)
F12—C12—F13	107.4 (3)		

Symmetry codes: (i) -x, -y+1, -z+1; (ii) -x+1, -y+1, -z+1.

S2. Microanalysis of Precursor (1)

NMR

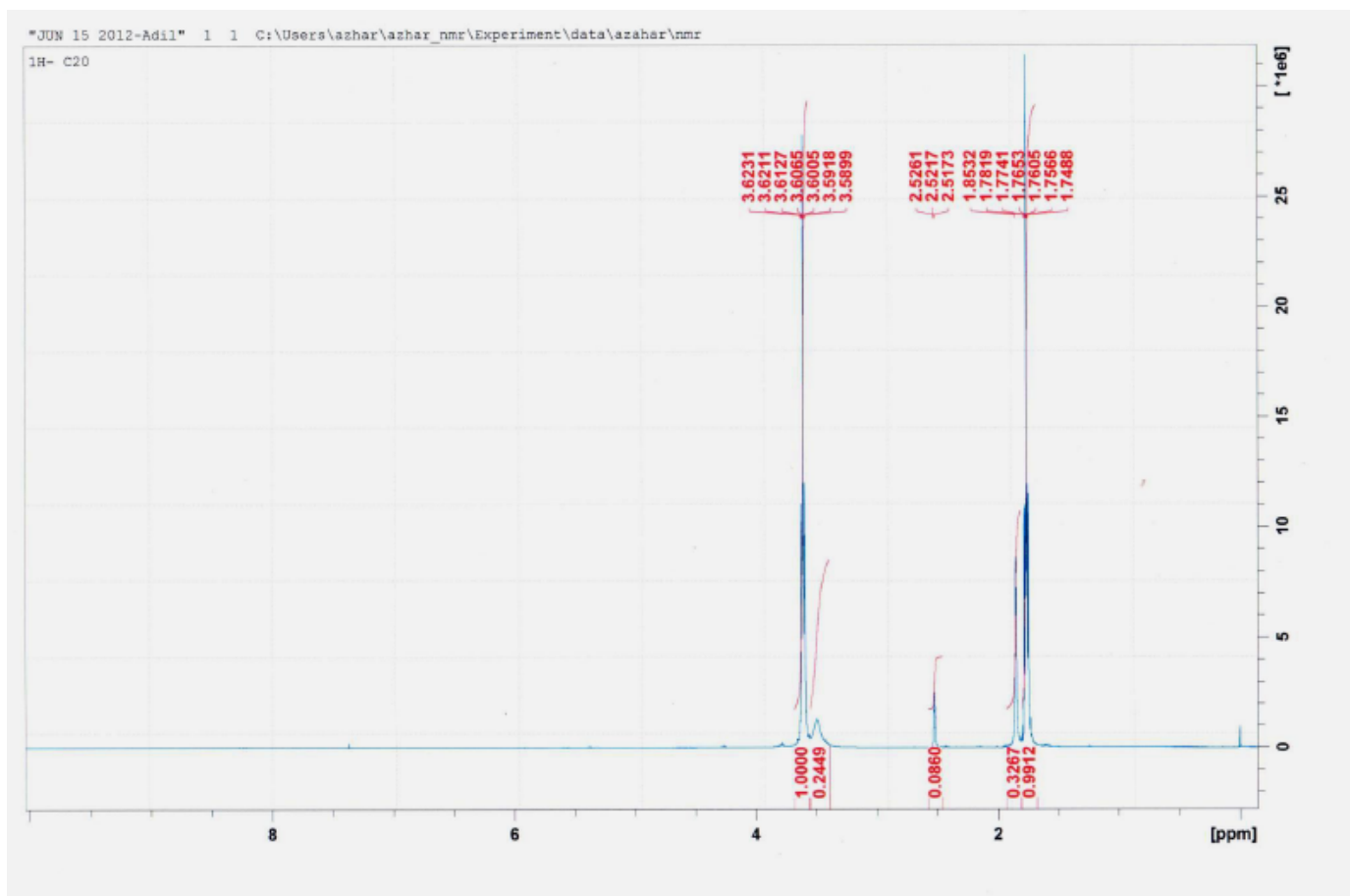


Fig. S1. ^1H -NMR of precursor (1)

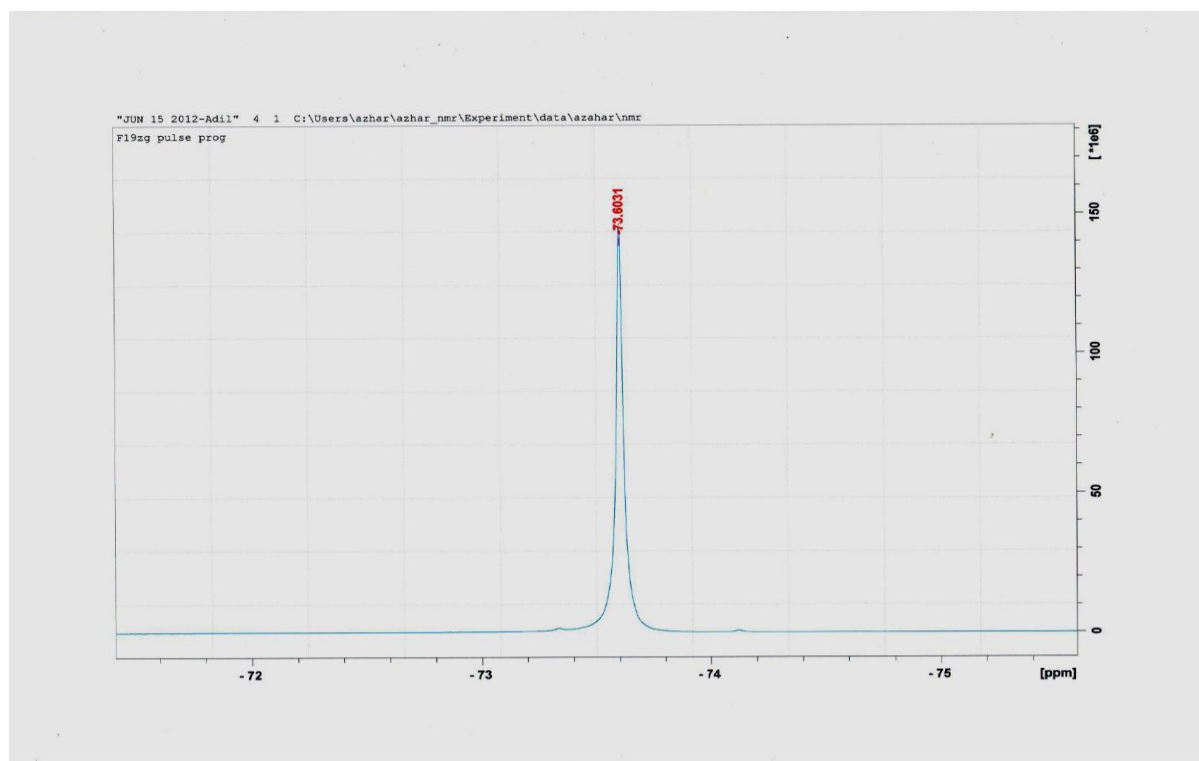


Fig. S2. ^{19}F -NMR of precursor (1)

FTIR

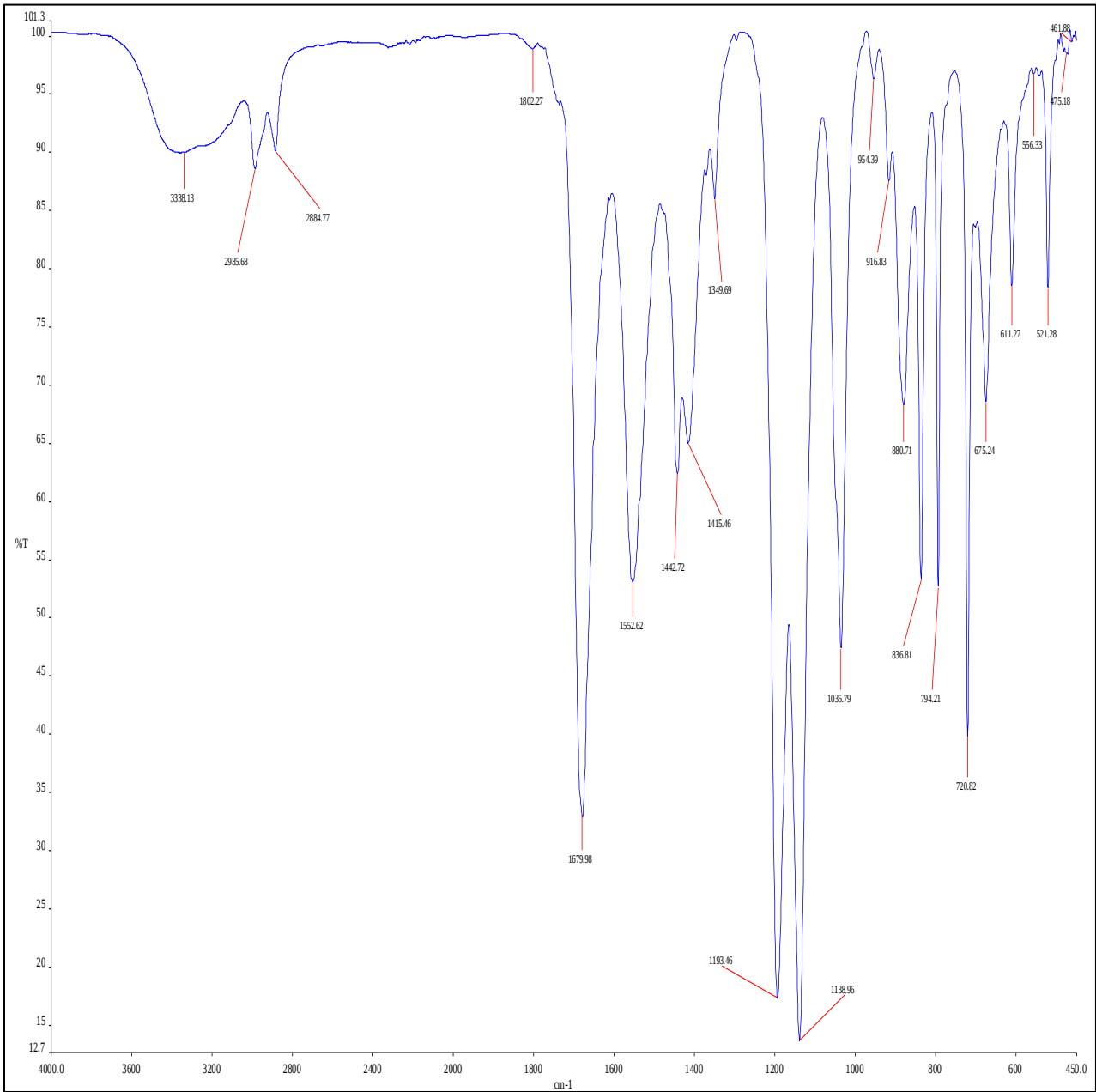


Fig. S3. FTIR of precursor (1)

S3. EDX and XRD of $\text{Zn}_{(1-x)}\text{Cd}_x\text{O}$ thin films

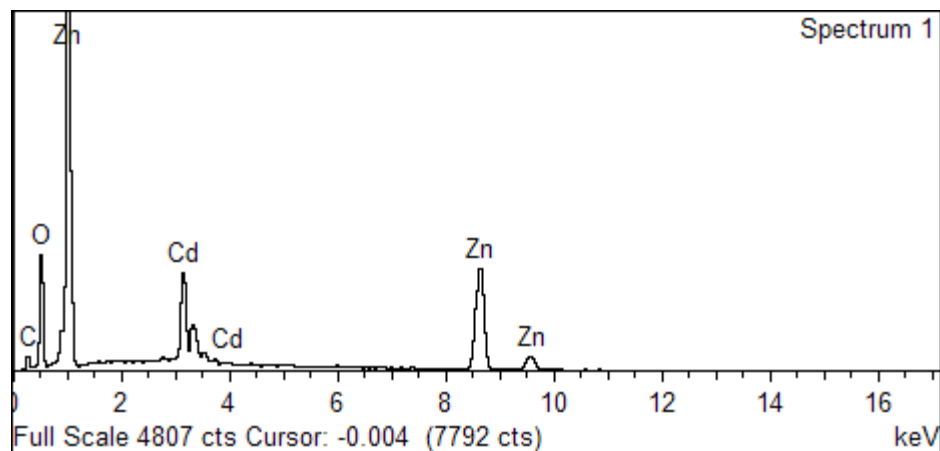


Fig. S4. EDX of $\text{Zn}_{0.85}\text{Cd}_{0.15}\text{O}$ thin films formed from methanol.

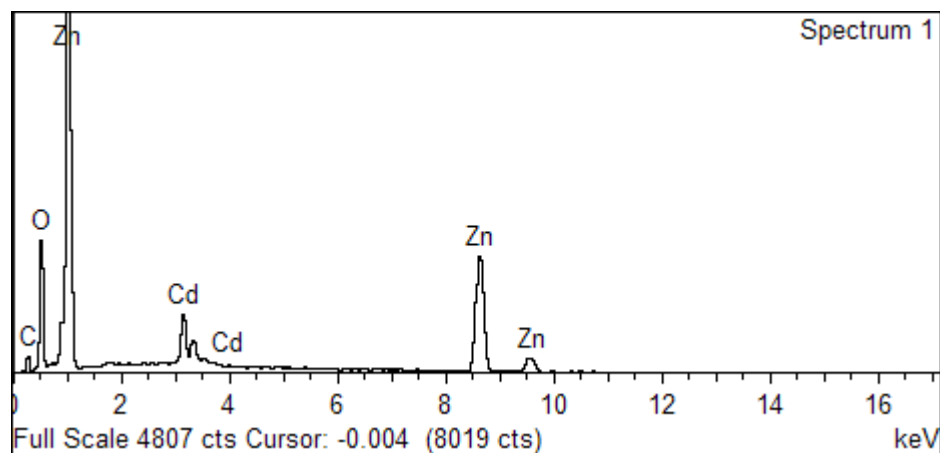


Fig. S5. EDX of $\text{Zn}_{0.92}\text{Cd}_{0.08}\text{O}$ thin films formed from ethanol.

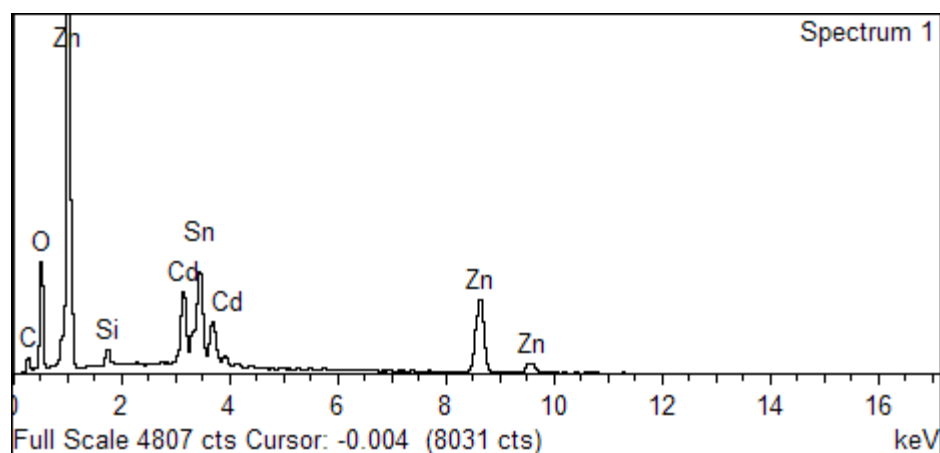


Fig. S6. EDX of $\text{Zn}_{0.83}\text{Cd}_{0.17}\text{O}$ thin films formed from

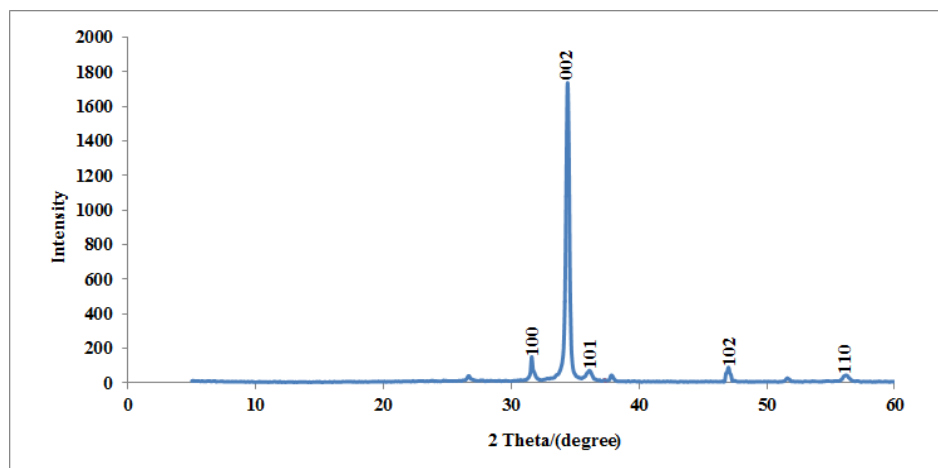


Fig. S7. Powder X-ray diffraction of Zn_{0.92}Cd_{0.08}O thin films formed from ethanol

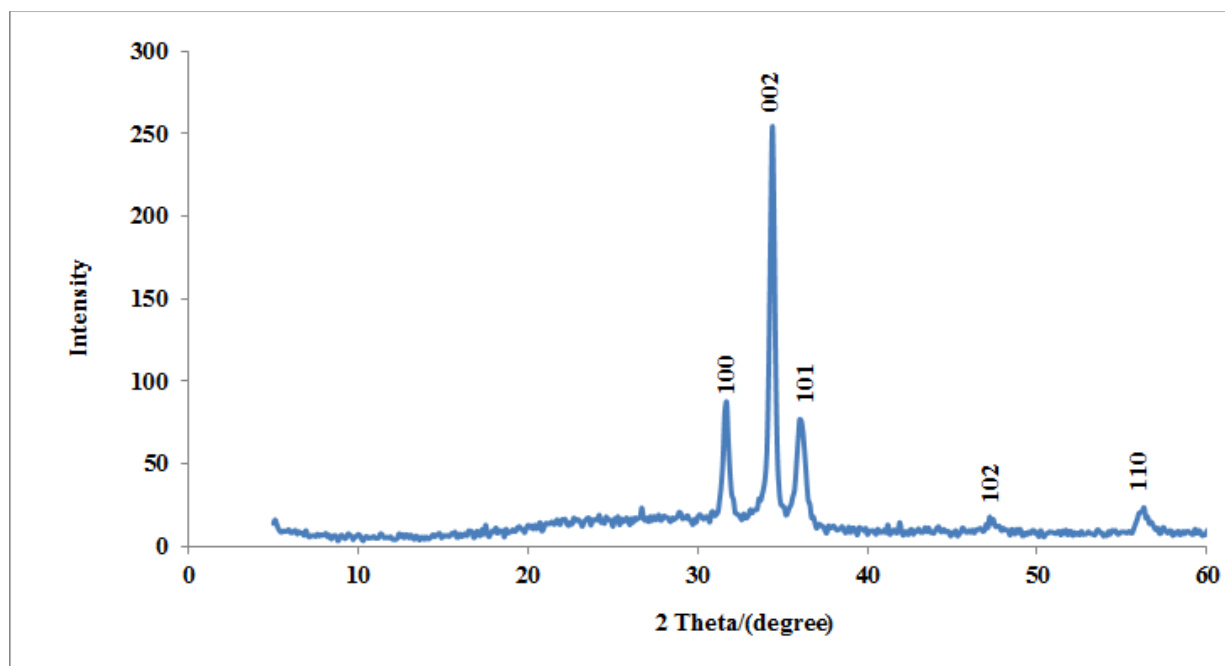


Fig. S8. Powder X-ray diffraction of Zn_{0.85}Cd_{0.15}O thin films formed from methanol