Supporting Information

Contents

Table **S1**: List of conductivity of some of the reported conductive MOFs in assynthesized, guest-free and iodine-loaded forms.

MOFs	Assynthesized/ solvated Conductivity (Scm^{-1})	Guest-free/ desolvated Conductivity (Scm^{-1})	I_2 loaded conductivity (Scm^{-1})	Measurments	E_a (eV)	References
$Co_2(DOBDC)(DMF)_2$	-	1.5×10^{-13}	-	2-probe	0.58	1
$Ni_2(DOBDC)(DMF)_2$	-	2.8×10^{-14}	-	2-probe	0.62	
$Zn_2(DOBDC)(DMF)_2$	-	3.3×10^{-14}	-	2-probe	0.54	
$Mn_2(DOBDC)(DMF)_2$	3.9×10^{-13}	3.0×10^{-13}	-	2-probe	0.55	2
$Mn_2(DSBDC)(DMF)_2$	2.5×10^{-12}	1.2×10^{-12}	-	2-probe	0.81	3
$Cu [Ni(pdt)_2]$	-	1×10^{-8}	1×10^{-4}	2-probe	-	4
$[Co(ebic)_2]_n$	-	2.46×10^{-9}	2.21×10^{-7}	-	-	5
$[Zn(ebic)_2]_n$	-	4.33×10^{-9}	3.47×10^{-7}	-	-	
$[Co_{1.5}(bdc)_{1.5}(H_2bpz)]$	-	2.59×10^{-9}	1.56×10^{-6}	2-probe	-	6
$[Tb_3(Cu_4I_4)_3(ina)_9]_n$	-	5.72×10^{-11}	2.16×10^{-4}	-	-	7
Cu_3HIB_2	13	-	-	4-probe	-	8
Ni_3HIB_2	8	-	-	4-probe	-	
Ni_3HTB_2	0.15	-	-	2-probe	-	9
Ni_3HITP_2	2	-	-	2-probe	-	10
$[Cu_3(C_6S_6)]_n$	1,580	-	-	4-probe	0.00206	11
Cu_3BHS	110	-	-	4-probe	-	12
Cu_3HHTP_2	1.5	-	-	4-probe	-	13
Cu-CAT-1	0.18	-	-	4-point	-	14
Ni_3TTB_2	0.1	-	-	van der Pauw	0.041	15
$[H_2N(CH_3)_2][Mn(HCO_2)_3]$	4.237×10^{-1}	5.279×10^{-1}	-	2-probe	0.00731	This work
$[H_2N(CH_3)_2][Co(HCO_2)_3]$	3.015×10^{-1}	1.052×10^{-1}	-	2-probe	0.01305	
$[H_2N(CH_3)_2][Ni(HCO_2)_3]$	4.872×10^{-3}	4.975×10^{-1}	-	2-probe	0.01590	
$[H_2N(CH_3)_2][Zn(HCO_2)_3]$	4.785×10^{-3}	1.492×10^{-1}	-	2-probe	0.01599	

H_2pdt = pyrazine- 2,3-dithiol, Hebic = 2-ethyl-1H-benzo[d]imidazole-5-carboxylic acid, H_2bdc = benzene-1,4-dicarboxylic acid, bpz = 3,3,5,5-tetramethyl-4,4-bipyrazole, Hina = isonicotinic acid, DOBDC= 2,5-dioxybenzene-1,4-dicarboxylate, DSBDC= 2,5-disulfidobenzene-1,4-dicarboxylate, HIB= Hexaiminobenzene, HTB= Hexathiolbenzene, HITP=2,3,6,7,10,11-Hexaiminotriphenylene, BHS= Benzenehexaselenolate, HHTP= 2,3,6,7,10,11-hexahydroxytriphenylene, CAT= Catecholate, TTB= triamino-trithiolbenzene, E_a = activation energy.
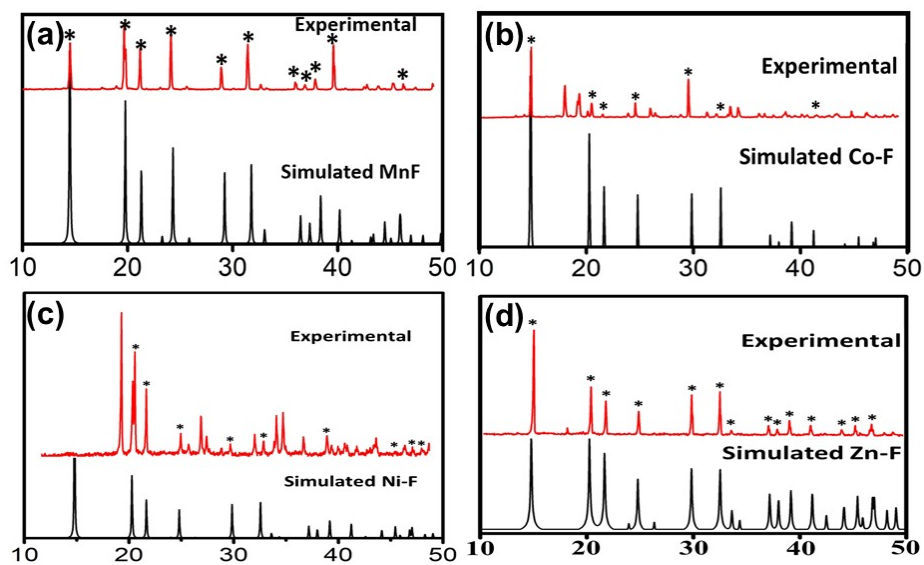
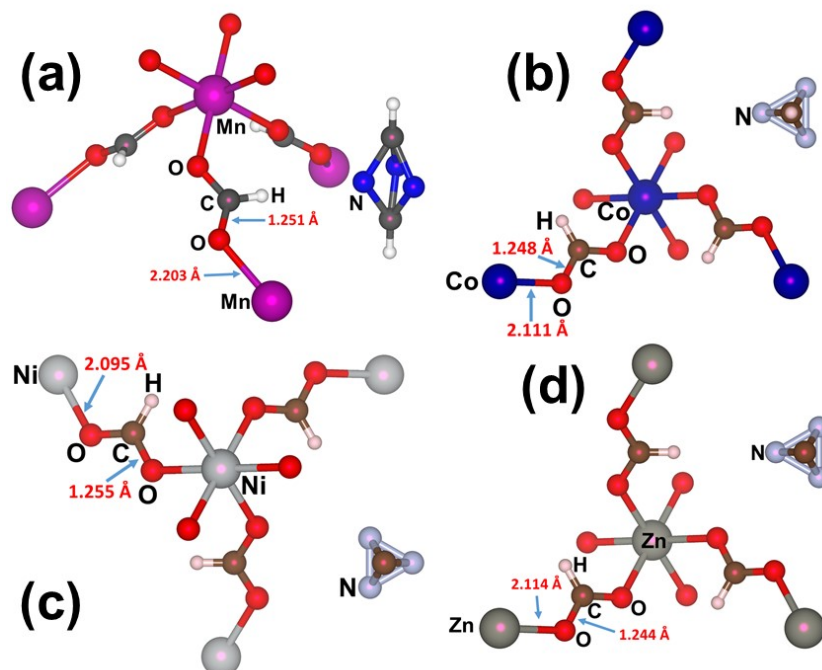Fig **S1**: PXRD of (a) Mn-F, (b) Co-F, (c) Ni-F and (d) Zn-F MOFs; simulated (black) and experimental (red).

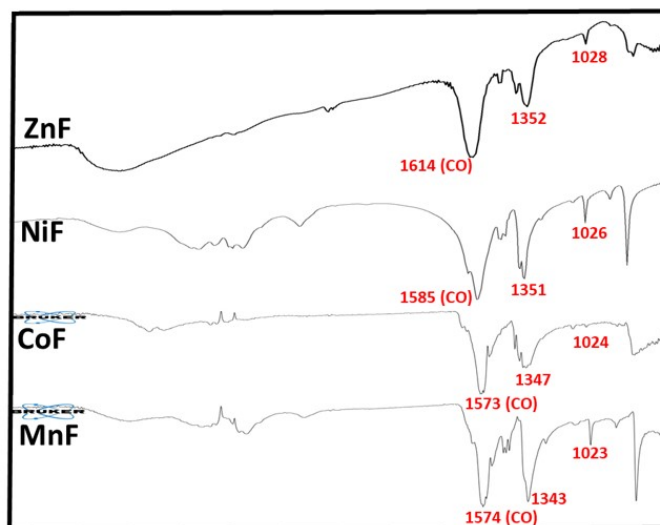Fig **S2**: M-O and C-O bond lengths of (a) **Mn-F**, (b) **Co-F**, (c) Ni-F and (d) **Zn-F**.

Fig **S3**: FTIR spectra of **Mn-F**, **Co-F**, **Ni-F** and **Zn-F** MOFs.
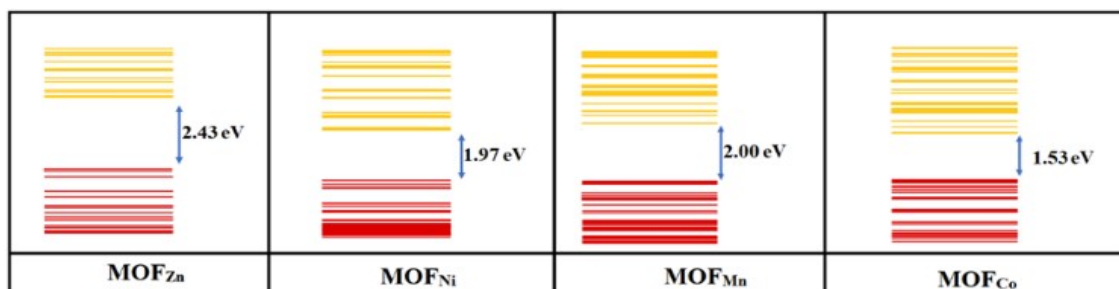

Fig **S4:** Calculated band gap (eV) of the MOFs.

Table **S2**: CO stretching frequency values of MOFs after and before heating.

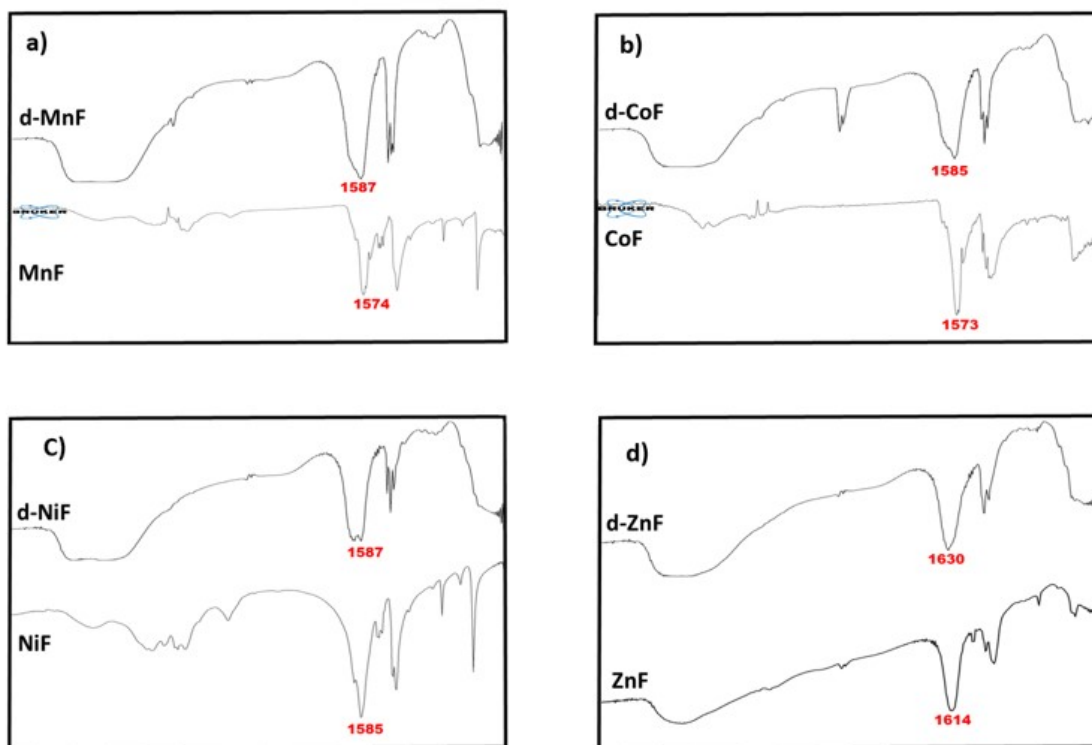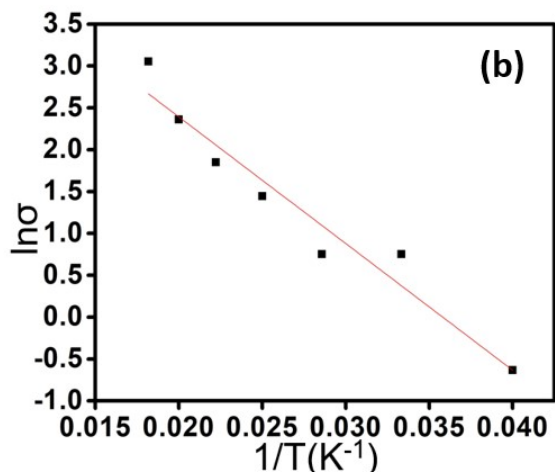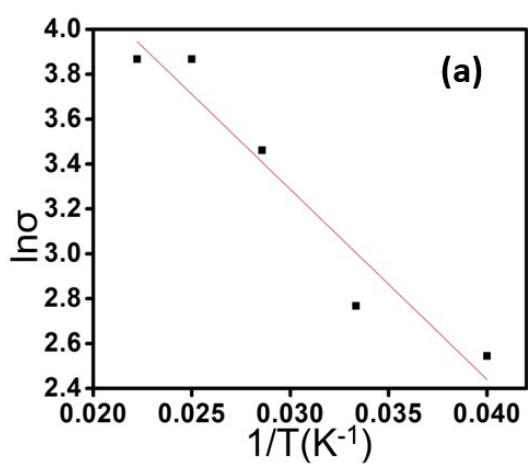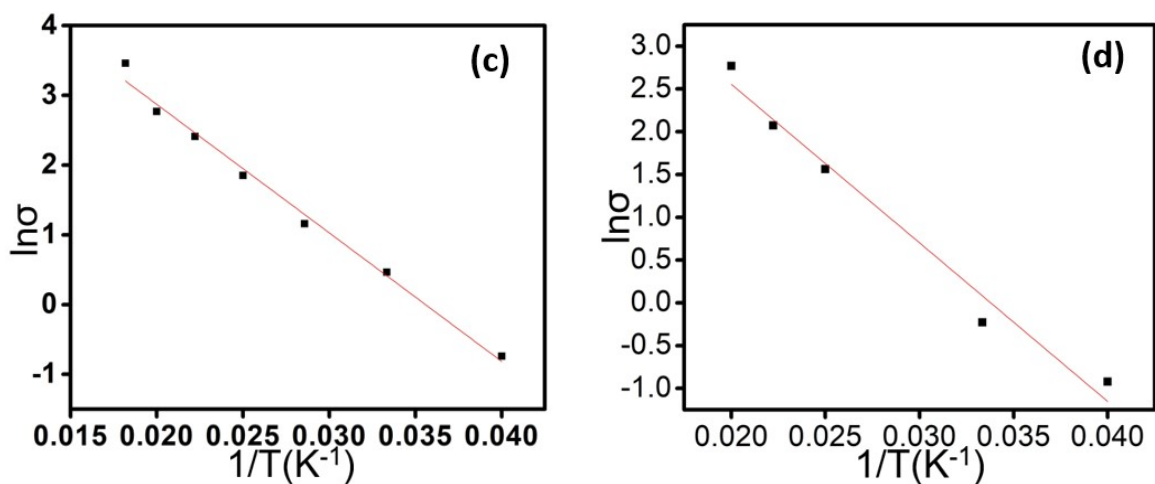| MOF	Before heating, ϑ_{co} in cm^{-1}	After heating, ϑ_{co} in cm^{-1}
Mn-F	1574	1587
Co-F	1573	1585
Ni-F	1585	1587
Zn-F	1614	1630

Figure **S5**: FTIR spectra C-O stretching frequencies before and after heating in (a) **Mn-F**, (b) **Co-F**, (c) **Ni-F** and (d) **Zn-F**.

Fig S6: Temperature dependent conductivity curve of (a) **Mn-F**, (b) **Co-F**, (c) **Ni-F** and (d) **Zn-F** MOFs.
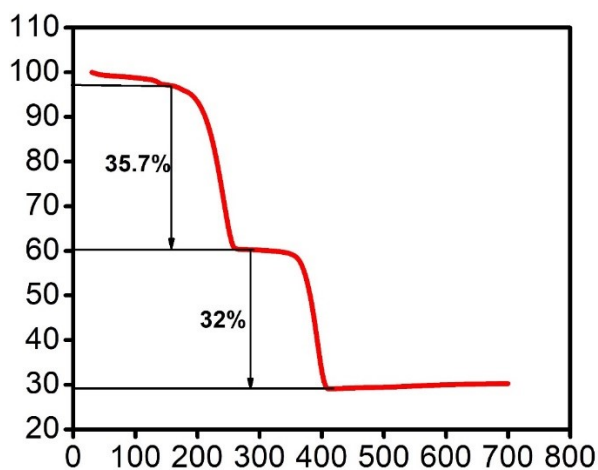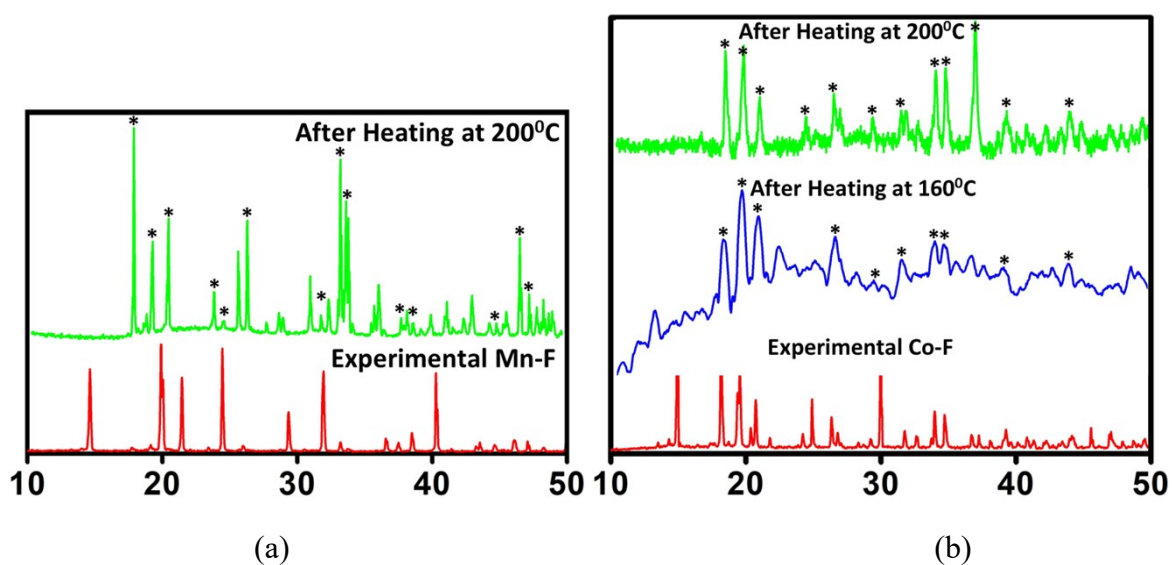

Fig **S7**: TGA graph of **Mn-F**.

Fig **S8**: PXRD of (a) **Mn-F** and (b) **Co-F** before and after heating.
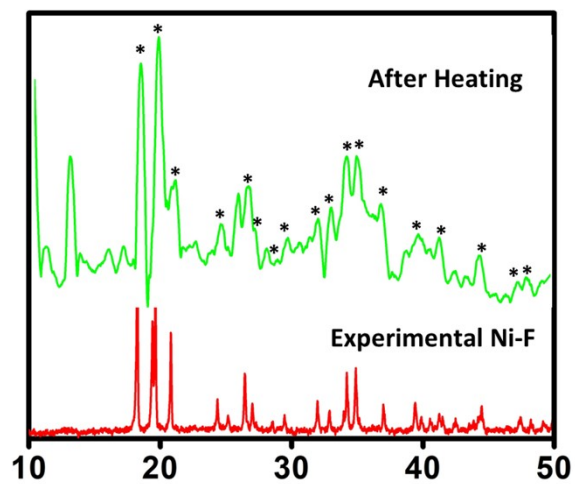
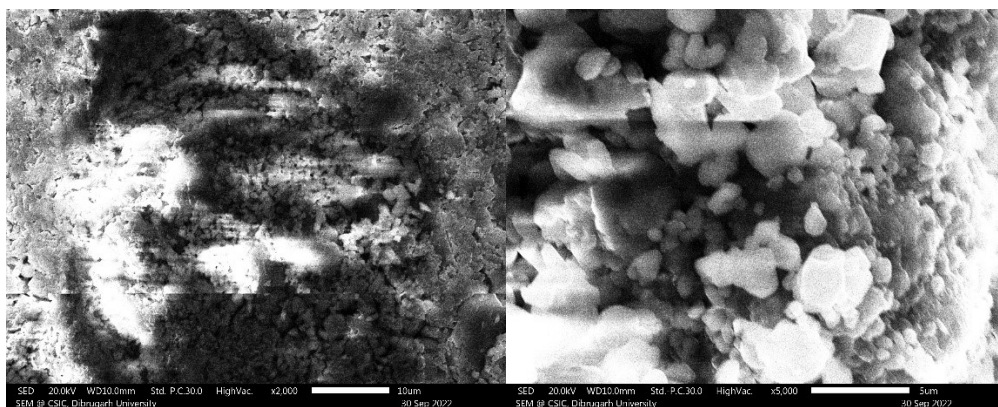Fig **S9**: PXRD of **Ni-F**; simulated (black) and after heat (green) at 160 ºC for 24 h.

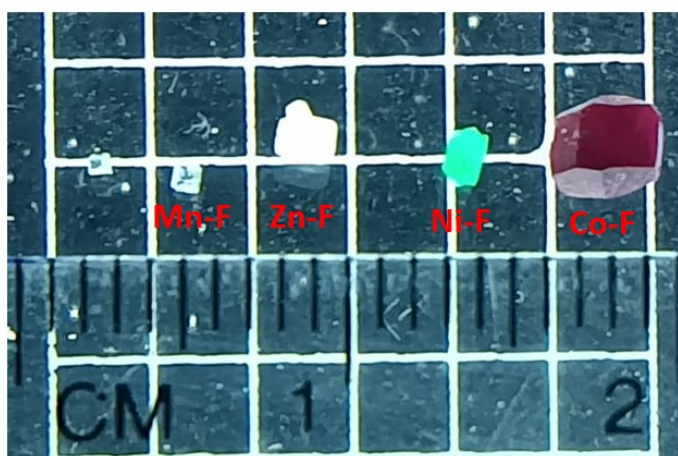Figure **S10**: SEM image (2000X and 5000X) of the **Co-F** pellet.

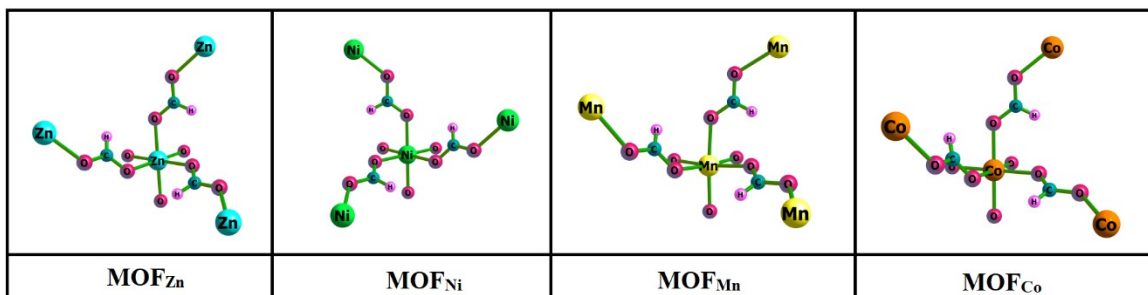Fig **S11:** Single crystal images of the MOFs.

Fig **S12**: Optimized geometries of the Zn, Ni, Mn and Co containing Metal-Organic Frameworks.

Table **S3**: Crystallographic table

Compound No.	**Mn-F**	**Co-F**	**Zn-F**
Formulae	$C_{15}H_{15}Mn_3N_9O_{18}$	$C_{15}H_9Co_3N_9O_{18}$	$C_{15}H_9N_9O_{18}Zn_3$
Mol. wt.	774.18	774.10	799.48
CCDC No	2263898	2263917	2263916
Crystal system	Trigonal	Trigonal	Trigonal
Space group	*R-3c*	*R-3c*	*R-3c*
Temperature (K)	298 (2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073
a (Å)	8.3840(16)	8.1984(6)	8.1966(4)
b (Å)	8.3840(16)	8.1984(6)	8.1966(4)
c (Å)	23.021(6)	22.2560(17)	22.280(2)
α (°)	90.00	90.00	90.00
β (°)	90.00	90.00	90.00
γ (°)	120.00	120.00	120.00
V (Å³)	1295.50(17)	1295.50(17)	1296.32(15)
Z	2	2	2
Density/gcm⁻³	1.897	1.984	2.048
Abs. Coeff. /mm⁻¹	1.428	1.447	2.884
Abs. correction	none	none	none
F(000)	768	672	792

Total no. of reflections	279	268	267
Reflections, $I > 2\sigma(I)$	277	267	263
Max. 2θ (°)	25.24	25.21	25.13
Ranges (h, k, l)	-10≤ h ≤10 -10 ≤ k ≤10 -27 ≤ 1 ≤ 27	-9≤ h ≤9 -9 ≤ k ≤9 -26 ≤ 1 ≤ 26	-9≤ h ≤9 -9 ≤ k ≤9 -25 ≤ 1 ≤ 26
Completeness to 2θ (%)	0.976	1.000	1.000
Data/ Restraints / Parameters	279/0/ 28	268/0/ 25	267/0/ 25
Goof (F^2)	1.262	1.168	1.065
R indices [$I > 2\sigma(I)$]	0.0729	0.0553	0.0750
R indices (all data)	0.0730	0.0552	0.0755

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