Supporting Information

2D and 3D coordination polymers involving trigonal tritopic linker

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General remarks

Powder X-ray diffraction (PXRD) patterns were obtained in transmission geometry using a STOE StadiP X-ray diffractometer equipped with an IPDS detector and monochromated Cu-Kα1 (λ = 0.15405 nm) radiation (40 kV, 30 mA). Thermogravimetric analyses (TG) were carried out under air atmosphere using a Netzsch STA 409 thermal analyzer. Infrared spectra (IR) were recorded in diffuse reflection geometry using a BIORAD Excalibur FTS3000 (Varian Inc.) infrared spectrometer. Elemental analysis (C, H, N) was performed with a EA 3000 Euro Vector CHNSO analyzer from Hekatech.

Preparation and characterization of 4,4',4''-(benzene-1,3,5-triyl-tris(benzene-4,1-diyl))tribenzoic acid (H_3BBC)

A mixture of 4-acetyl-4'-bromobiphenyl (13.2 g, 48.0 mmol) and trifluoromethanesulfonic acid (2.4 mL) in toluene (100 mL) was heated to reflux under argon atmosphere for 14 h. The formed precipitate was filtered off, washed with methanol and re-crystallized from chloroform. After drying at 80 °C 4.9 g (13.3 %) of the product were obtained.[1]

^{1}H-NMR ($CDCl_3$): δ/ppm = 7.53 (d, 6H), 7.59 (d, 6H), 7.69 (d, 6H), 7.79 (d, 6H), 7.86 (s, 3H). ^{13}C-NMR ($CDCl_3$): δ/ppm = 121.76, 125.10, 127.44, 127.86, 128.65, 131.99, 139.31, 139.49, 140.29, 141.90. Elemental analysis for $C_{42}H_{27}Br_3$: calc. (%): C 65.40, H 3.53; found (%): C 65.27, H 3.30. IR: ν/cm^{-1} = 3088 (w), 3032 (w), 1598 (m), 1514 (w), 1484 (m), 1445 (m), 1390 (m), 1073 (m), 1001 (s), 854 (m), 844 (m), 802 (s), 740 (m), 700 (m).

To a solution of 1,3,5-tris(4´-bromobiphenyl-4-yl)benzene (2.01 g, 2.61 mmol) in dry THF (120 mL), *n*-butyllithium (6.3 mL, 2.5 mol L^{-1} solution in hexane) was added slowly at -70 °C under argon atmosphere. After stirring the solution for 6 h at 203K, CO_2 gas was passed through the reaction mixture for 30 min. After the solution was warmed up to room temperature under CO_2 flow, water was added to remove the excess of *n*-BuLi. Acidifying the solution with acetic acid gave a clear solution. The THF

was removed under reduced pressure and the resulting white precipitate was collected by filtration. Drying the substance under vacuum yields 1.66 g (95.4 %) of the product.[2]

^{1}H-NMR (DMSO): δ/ppm = 7.90 (d, 12H), 8.06 (m, 15H), 12.98 (s, 3H). ^{13}C-NMR (DMSO): δ/ppm = 124.61, 126.85, 127.60, 128.01, 129.78, 130.12, 138.39, 139.94, 141.13, 143.83, 167.23. Elemental analysis for $C_{45}H_{30}O_6 \cdot 1.5\ H_2O$: calc. (%): C 77.91, H 4.79; found (%): C 78.10, H 4.63. IR: ν/cm^{-1} = 3032 (w), 2966 (w), 1681 (s), 1605 (s), 1574 (w), 1552 (w), 1527 (m), 1495 (m), 1422 (m), 1391 (m), 1281 (s), 1178 (m), 1124 (m), 1004 (m), 937 (w), 866 (m), 822 (s), 771 (s), 733 (m), 697 (m), 664 (w).

X-ray powder diffraction experiments and thermogravimetric analyses

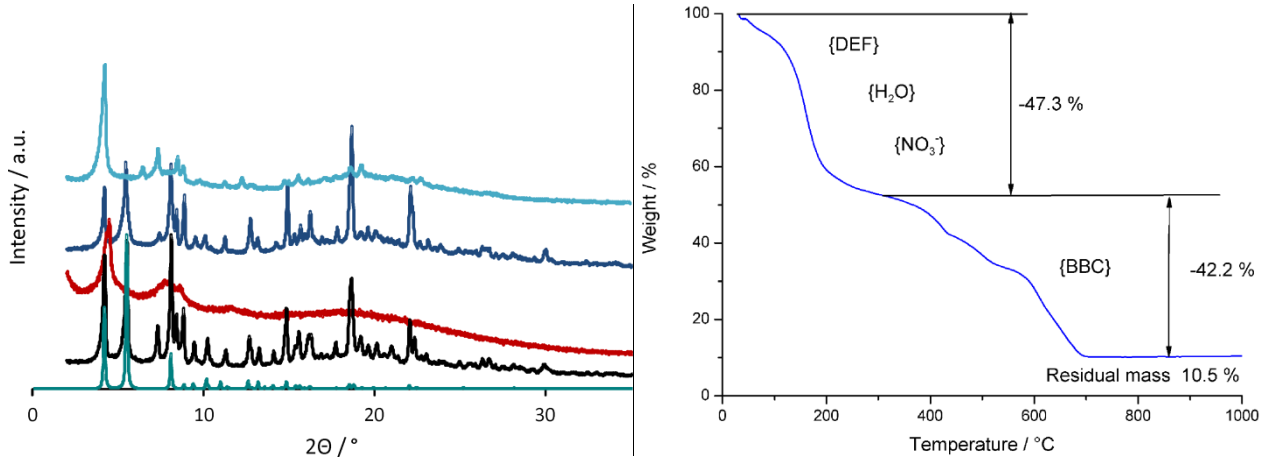


Figure S1. *left:* PXRD patterns of DUT-40: calculated (green), as synthesized (black), activated by supercritical CO_2 drying (red), resolvated with liquid DMF (dark blue), and resolvated with DMF vapor (light blue); *right:* Thermogravimetric analysis of DUT-40 (as synthesized).

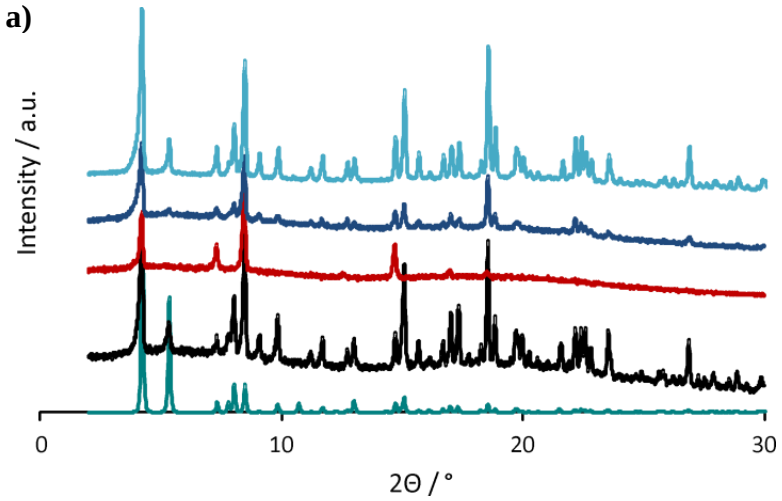


Figure S2. a) PXRD patterns of DUT-42: calculated (green), as synthesized (black), activated by supercritical CO_2 drying (red), resolvated with liquid DMF (dark blue), and resolvated with DMF vapor (light blue).

b)

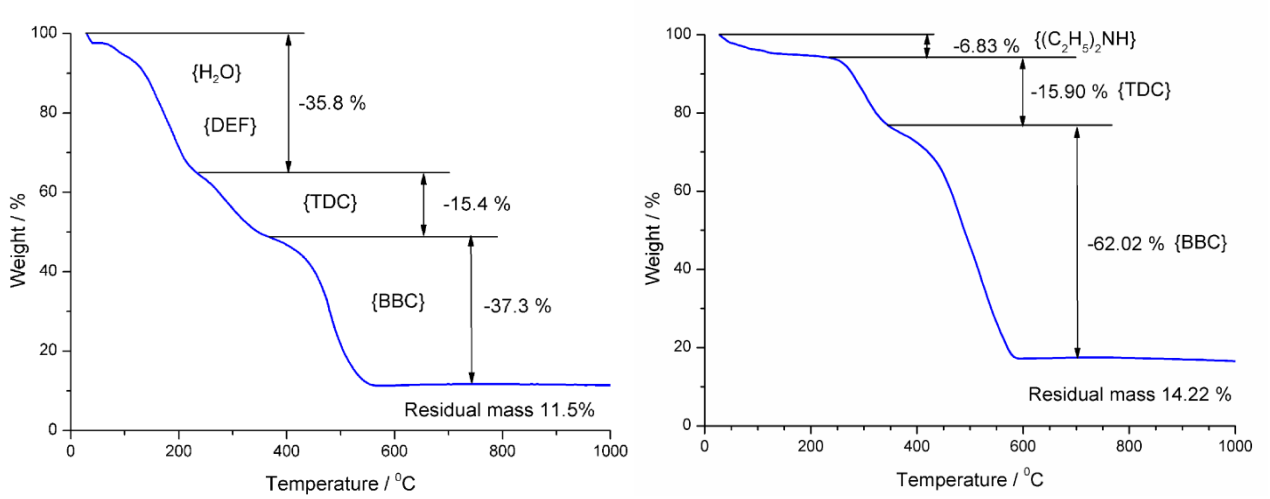


Figure S3. b) *left:* Thermogravimetric analysis of as synthesized DUT-42; *right*: Thermogravimetric analisis of DUT-42 sample after supercritical CO_2 drying).

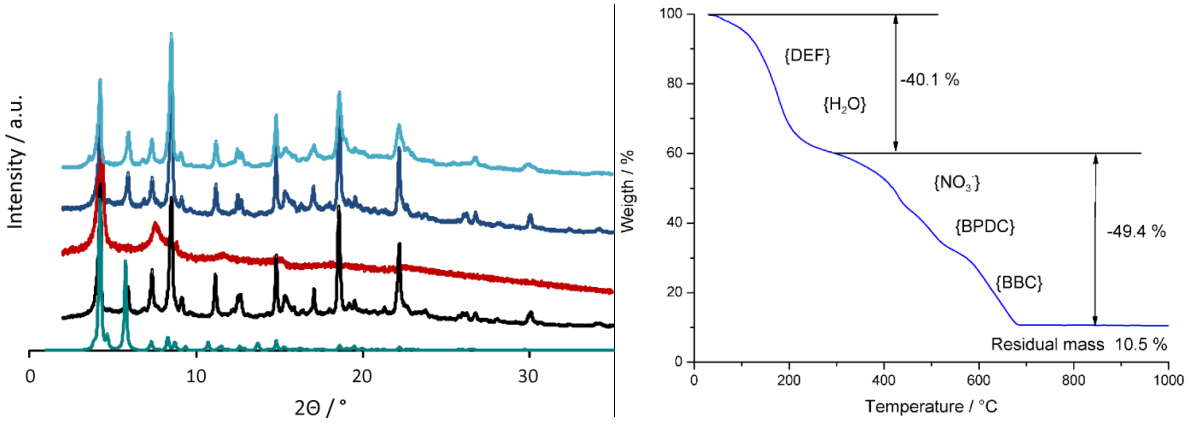


Figure S4. *left:* PXRD patterns of DUT-43: calculated (green), as synthesized (black), activated by supercritical CO_2 drying (red), resolvated with liquid DMF (dark blue), and resolvated with DMF vapor (pale blue); *right:* Thermogravimetric analysis of DUT-43 (as synthesized).

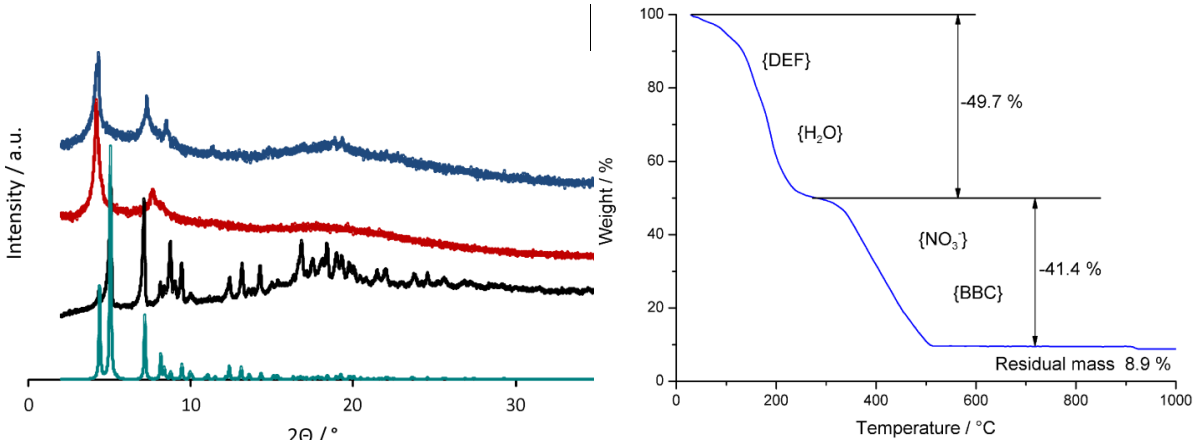
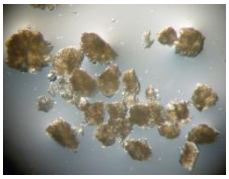
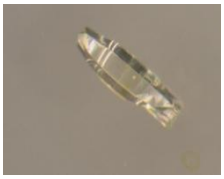
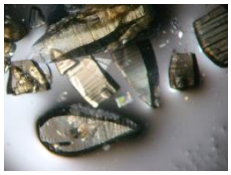
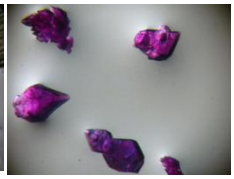
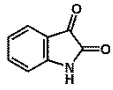
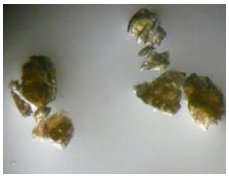
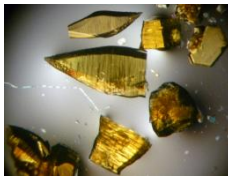
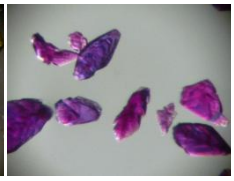
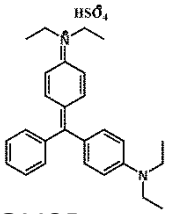
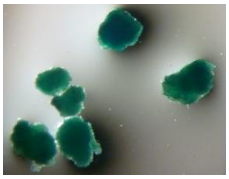
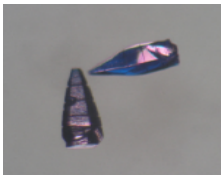
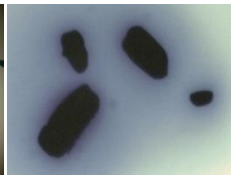
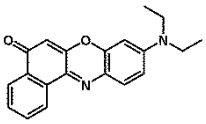
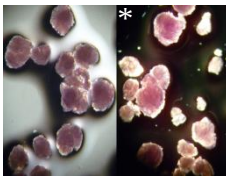
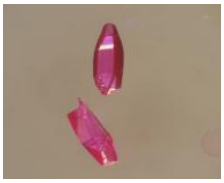
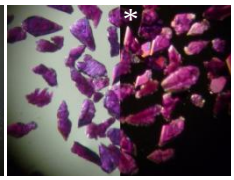
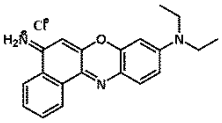
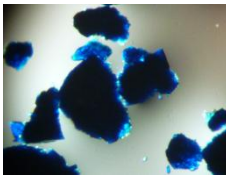
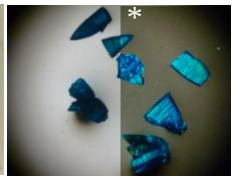
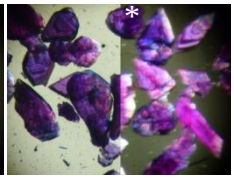
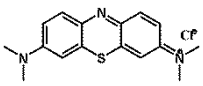
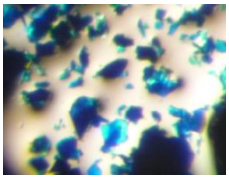
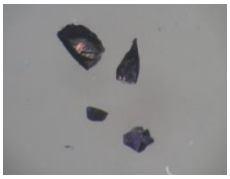
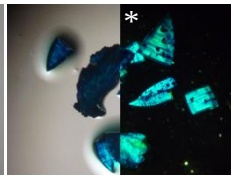
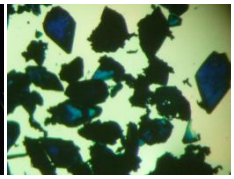
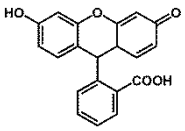
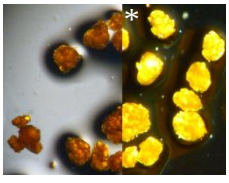
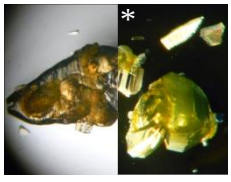
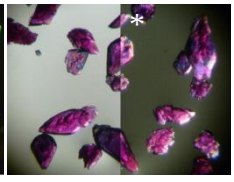


Figure S5. *left:* PXRD patterns of DUT-44: calculated (green), as synthesized (black), activated by supercritical CO_2 drying (red), and resolvated with DEF (blue); *right:* Thermogravimetric analysis of DUT-44 (as synthesized).

Adsorption of dyes

Table S1. Dye adsorption of DUT-40 and DUT-42 – 44.

	DUT-40	DUT-42	DUT-43	DUT-44
as made compound				
Isatin @MOF 				
Brilliant green@MOF 				
Nile red@MOF 				
Nile blue@MOF 				
Methylene blue@MOF 				
Fluorescein@MOF 				

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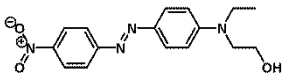

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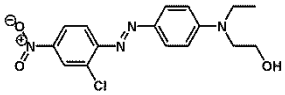

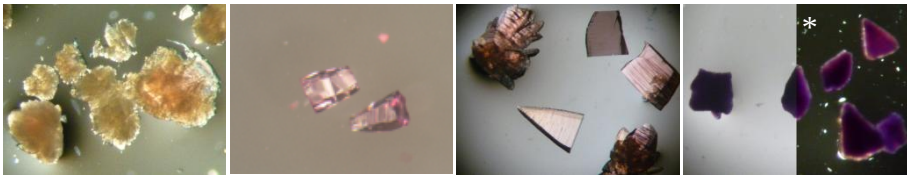

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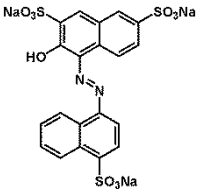

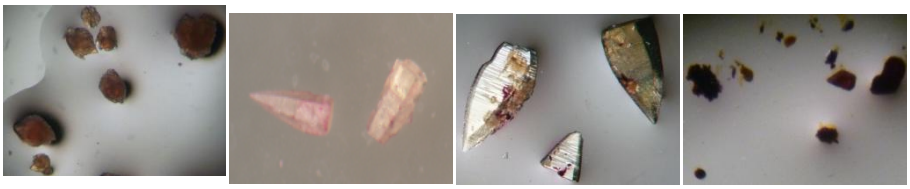

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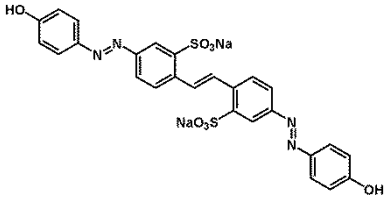

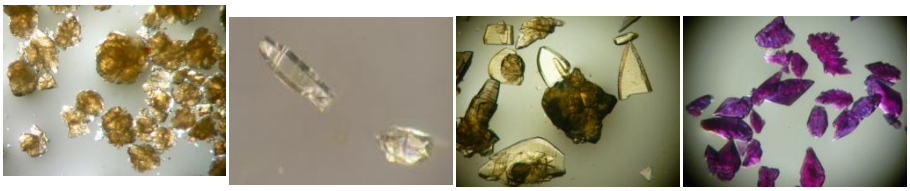

* The picture was taken thought the polarizing filter of the microscope.

Crystallographic study

Table S2. Crystallographic experimental data for compounds **1-5**.

Compound	**1** **DUT-40**	**2** **DUT-41**	**3** **DUT-42**	**4** **DUT-43**	**5** **DUT-44**
Empirical formula	$C_{45}H_{27}O_8Zn_2$	$C_{90}H_{54}O_{15}Zn_3$	$C_{51}H_{29}O_{10}SZn_2$	$C_{273}H_{195}N_4O_{52}Zn_{10}$	$C_{55}H_{49}Co_2N_3O_{12}$
Formula weight	826.41	1571.44	964.54	5017.03	1061.83
Crystal system Space group	Monoclinic *C*2/*c*	Monoclinic *Cc*	Hexagonal $P6_522$	Monoclinic *C*2/*c*	Monoclinic *C*2/*c*
Unit cell dimensions / Å, deg.	a = 19.834(4) b = 42.111(8) c = 12.913(3) β = 118.69(3)	a = 24.127(5) b = 41.811(8) c = 20.186(4) β = 115.27(3)	a = 24.057(3) c = 26.996(5)	a = 23.934(5) b = 41.860(8) c = 45.532(9) β = 90.12(3)	a = 39.776(8) b = 24.693(5) c = 21.823(4) β = 117.94(3)
Volume / $Å^3$	9461(3)	18414(6)	13530(3)	45617(16)	18936(6)
Z, Calc. density / Mg/m^3	4, 0.580	4, 0.567	6, 0.710	4, 0.731	8, 0.745
μ / mm^{-1}	0.952	0.747	1.053	0.558	0.386
F(000)	1684	3216	2946	10308	4400
Limiting indices	-24≤h≤24 -53≤k≤53 -17≤l≤17	-31≤h≤32 -53≤k≤52 -25≤l≤25	-30≤h≤30 -31≤k≤31 -33≤l≤33	-23≤h≤23 -48≤k≤47 -52≤l≤52	-42≤h≤41 -28≤k≤28 -25≤l≤25
Reflections collected / unique	47983/10707 R(int)=0.0838	96110/40518 [R(int)=0.0544]	155346/11149 [R(int)=0.0934]	132373/32809 [R(int)=0.0584]	57847/13628 [R(int)=0.0344]
Data / parameters	10707/252	40518/963	11149/293	32809/1534	13628/650
GooF on F^2	0.845	0.912	1.061	1.129	1.086
R $[I>2\sigma(I)]$*	R_1=0.0703 wR_2=0.1866	R_1=0.0567 wR_2=0.1484	R_1=0.0428 wR_2=0.1086	R_1=0.0911 wR_2=0.2671	R_1=0.0702 wR_2=0.2145
R (all data)*	R_1=0.1311 wR_2=0.2089	R_1=0.0710 wR_2=0.1576	R_1=0.0524 wR_2=0.1150	R_1=0.1066 wR_2=0.2840	R_1=0.0787 wR_2=0.2242
Flack x parameter	-	0.448(4)**	0.041(6)	-	-
Solvent accessible void / % ($Å^3$)	67.8 (6415)	67.5 (12429)	60.9 (8240)	56.7 (25865) 62.9 (28687)***	54.9 (10396)
Number of electron counted in void (per unit cell)	1296	4248	3200	5490 7084***	1417
Largest diff. peak / hole, e/$Å^3$	0.871 / -0.410	0.622 / -0.528	0.830 / -0.551	1.236 / -1.797	0.917 / -0.389

*$R1 = \Sigma(F_o - F_c)/\Sigma F_o$; $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

**The value of Flack parameter indicates that absolute configuration cannot be determined for DUT-41 structure. Thus, the structure was refined as racemic twin.

***Solvent accessible void and electrons count after removing all solvent molecules.

Table S3. Selected geometrical parameters for DUT-40.

	Bond length / Å		Angle / deg.
Zn(1)-O(1)	1.931(3)	O(1)-Zn(1)-O(2)#1	123.90(13)
Zn(1)-O(2)#1	1.951(2)	O(1)-Zn(1)-O(3)#2	106.16(13)
Zn(1)-O(3)#2	1.963(2)	O(2)#1-Zn(1)-O(3)#2	104.91(11)
Zn(1)-O(4)	2.164(2)	O(1)-Zn(1)-O(4)	105.19(13)
		O(2)#1-Zn(1)-O(4)	108.18(10)
		O(3)#2-Zn(1)-O(4)	107.68(10)

Symmetry transformations used to generate equivalent atoms: [#1] -x+1/2,y-1/2,-z+5/2; [#2] x-1/2,y-1/2,z-1.

Table S4. Selected geometrical parameters for DUT-41.

Bond length	Å	Valence angle	deg.	Valence angle	deg.
Zn(1)-O(6)#1	2.249(3)	O(6)#1-Zn(1)-O(13)	168.9(3)	O(3)#2-Zn(2)-O(2)	113.05(9)
Zn(1)-O(13)	2.284(4)	O(6)#1-Zn(1)-O(4)#2	86.59(13)	O(5)#1-Zn(2)-O(2)	116.26(10)
Zn(1)-O(4)#2	2.321(3)	O(13)-Zn(1)-O(4)#2	83.0(3)	O(3)#2-Zn(2)-O(7)	96.66(11)
Zn(1)-O(1)	2.337(2)	O(6)#1-Zn(1)-O(1)	86.61(11)	O(5)#1-Zn(2)-O(7)	94.27(11)
Zn(1)-O(11)	2.354(2)	O(13)-Zn(1)-O(1)	96.59(16)	O(2)-Zn(2)-O(7)	99.77(9)
Zn(1)-O(8)	2.478(5)	O(4)#2-Zn(1)-O(1)	87.12(10)	O(9)-Zn(3)-O(12)	110.17(9)
Zn(2)-O(3)#2	1.9286(19)	O(6)#1-Zn(1)-O(11)	90.43(9)	O(9)-Zn(3)-O(10)	93.91(15)
Zn(2)-O(5)#1	1.932(2)	O(13)-Zn(1)-O(11)	87.17(15)	O(12)-Zn(3)-O(10)	96.69(13)
Zn(2)-O(2)	1.9529(18)	O(4)#2-Zn(1)-O(11)	97.26(9)	O(9)-Zn(3)-O(14)#1	97.5(3)
Zn(2)-O(7)	2.067(2)	O(1)-Zn(1)-O(11)	174.57(9)	O(12)-Zn(3)-O(14)#1	139.6(3)
Zn(3)-O(9)	1.954(2)	O(6)#1-Zn(1)-O(8)	94.93(16)	O(10)-Zn(3)-O(14)#1	110.5(3)
Zn(3)-O(12)	1.9581(18)	O(13)-Zn(1)-O(8)	95.4(3)	O(9)-Zn(3)-O(15)#1	155.4(2)
Zn(3)-O(10)	2.081(5)	O(4)#2-Zn(1)-O(8)	177.63(14)	O(12)-Zn(3)-O(15)#1	91.0(2)
Zn(3)-O(14)#1	2.192(7)	O(1)-Zn(1)-O(8)	94.78(12)	O(10)-Zn(3)-O(15)#1	96.09(18)
Zn(3)-O(15)#1	2.293(7)	O(11)-Zn(1)-O(8)	80.93(12)	O(14)#1-Zn(3)-O(15)#1	57.9(2)
		O(3)#2-Zn(2)-O(5)#1	126.54(11)		

Symmetry transformations used to generate equivalent atoms: #1 x-1/2,y+1/2,z #2 x-1,y,z

Table S5. Selected geometrical parameters for DUT-42.

Bond length	Å	Valence angle	deg.
Zn(1)-O(5)	1.9367(14)	O(5)-Zn(1)-O(4)	121.95(9)
Zn(1)-O(4)	1.9475(16)	O(5)-Zn(1)-O(1)	116.19(7)
Zn(1)-O(1)	1.9528(14)	O(4)-Zn(1)-O(1)	103.31(8)
Zn(1)-O(3)	1.9766(13)	O(5)-Zn(1)-O(3)	104.67(8)
		O(4)-Zn(1)-O(3)	106.29(9)
		O(1)-Zn(1)-O(3)	102.45(7)

Table S6. Selected geometrical parameters for DUT-43.

Bond length	Å	Valence angle	deg.	Valence angle	deg.
Zn(1)-O(8)	1.954(3)	O(8)-Zn(1)-O(13)	124.07(14)	O(21)#1-Zn(4)-O(23)#2	109.85(19)
Zn(1)-O(13)	1.976(3)	O(8)-Zn(1)-O(11)	100.69(13)	O(15)-Zn(4)-O(23)#2	108.0(2)
Zn(1)-O(11)	1.994(3)	O(13)-Zn(1)-O(11)	102.75(14)	O(21)#1-Zn(4)-O(24)	101.6(2)
Zn(1)-O(1)	1.994(3)	O(8)-Zn(1)-O(1)	112.77(13)	O(15)-Zn(4)-O(24)	97.7(2)
Zn(1)-O(2)	2.465(4)	O(13)-Zn(1)-O(1)	111.99(14)	O(23)#2-Zn(4)-O(24)	98.44(17)
Zn(2)-O(6)	1.949(3)	O(11)-Zn(1)-O(1)	100.05(14)	O(18)-Zn(5)-O(19)	70.4(8)
Zn(2)-O(7)	1.950(3)	O(8)-Zn(1)-O(2)	86.01(15)	O(18)-Zn(5)-O(17)	73.2(5)
Zn(2)-O(4)	1.953(3)	O(13)-Zn(1)-O(2)	90.18(15)	O(19)-Zn(5)-O(17)	111.6(4)
Zn(2)-O(5)	1.983(3)	O(11)-Zn(1)-O(2)	158.12(12)	O(18)-Zn(5)-O(20)#1	109.2(5)
Zn(3)-O(10)	1.902(3)	O(1)-Zn(1)-O(2)	58.41(13)	O(19)-Zn(5)-O(20)#1	77.7(4)
Zn(3)-O(12)	1.907(4)	O(6)-Zn(2)-O(7)	122.04(14)	O(17)-Zn(5)-O(20)#1	170.5(2)
Zn(3)-O(9)	1.957(3)	O(6)-Zn(2)-O(4)	111.60(13)	O(18)-Zn(5)-O(16)	117.5(4)
Zn(3)-O(14)	2.033(4)	O(7)-Zn(2)-O(4)	111.04(13)	O(19)-Zn(5)-O(16)	75.4(6)
Zn(4)-O(21)#1	1.903(4)	O(6)-Zn(2)-O(5)	104.64(14)	O(17)-Zn(5)-O(16)	73.3(3)
Zn(4)-O(15)	1.918(4)	O(7)-Zn(2)-O(5)	102.91(13)	O(20)#1-Zn(5)-O(16)	112.3(3)
Zn(4)-O(23)#2	1.966(4)	O(4)-Zn(2)-O(5)	101.94(13)	O(18)-Zn(5)-O(22)#2	104.9(4)
Zn(4)-O(24)	2.022(5)	O(10)-Zn(3)-O(12)	126.29(17)	O(19)-Zn(5)-O(22)#2	175.0(7)
Zn(5)-O(18)	1.634(11)	O(10)-Zn(3)-O(9)	106.54(16)	O(17)-Zn(5)-O(22)#2	64.79(17)
Zn(5)-O(19)	1.728(13)	O(12)-Zn(3)-O(9)	103.75(19)	O(20)#1-Zn(5)-O(22)#2	105.8(2)
Zn(5)-O(17)	1.802(3)	O(10)-Zn(3)-O(14)	107.87(16)	O(16)-Zn(5)-O(22)#2	106.1(3)
Zn(5)-O(20)#1	1.986(5)	O(12)-Zn(3)-O(14)	107.29(17)		
Zn(5)-O(16)	1.992(6)	O(9)-Zn(3)-O(14)	102.68(15)		
Zn(5)-O(22)#2	2.049(4)	O(21)#1-Zn(4)-O(15)	134.0(3)		

Symmetry transformations used to generate equivalent atoms: #1 x-1/2,y+1/2,z #2 x+1/2,y+1/2,z

Table S7. Selected geometrical parameters for DUT-44.

Bond length	Å	Valence angle	deg.	Valence angle	deg.	Valence angle	deg.
Co(1)-O(5)	1.988(2)	O(5)-Co(1)-O(3)	102.76(11)	O(11)-Co(1)-O(10)	57.87(13)	O(8)-Co(2)-O(7)	88.52(15)
Co(1)-O(3)	1.998(2)	O(5)-Co(1)-O(11)	102.90(11)	O(9)-Co(1)-O(10)	85.38(12)	O(4)-Co(2)-O(1)	90.89(9)
Co(1)-O(11)	2.081(3)	O(3)-Co(1)-O(11)	95.13(12)	O(1)-Co(1)-O(10)	98.54(12)	O(2)-Co(2)-O(1)	94.46(11)
Co(1)-O(9)	2.156(2)	O(5)-Co(1)-O(9)	154.94(11)	O(4)-Co(2)-O(2)	95.57(10)	O(6)-Co(2)-O(1)	90.81(11)
Co(1)-O(1)	2.202(3)	O(3)-Co(1)-O(9)	95.21(11)	O(4)-Co(2)-O(6)	176.16(12)	O(8)-Co(2)-O(1)	89.41(13)
Co(1)-O(10)	2.296(3)	O(11)-Co(1)-O(9)	92.61(11)	O(2)-Co(2)-O(6)	87.72(11)	O(7)-Co(2)-O(1)	177.74(11)
Co(2)-O(4)	2.047(2)	O(5)-Co(1)-O(1)	98.45(10)	O(4)-Co(2)-O(8)	90.80(14)	O(8)-Co(2)-O(7)	88.52(15)
Co(2)-O(2)	2.058(3)	O(3)-Co(1)-O(1)	105.06(10)	O(2)-Co(2)-O(8)	172.48(13)		
Co(2)-O(6)	2.087(3)	O(11)-Co(1)-O(1)	146.47(10)	O(6)-Co(2)-O(8)	85.78(15)		
Co(2)-O(8)	2.095(3)	O(9)-Co(1)-O(1)	59.59(9)	O(4)-Co(2)-O(7)	88.24(10)		
Co(2)-O(7)	2.109(3)	O(5)-Co(1)-O(10)	86.39(12)	O(2)-Co(2)-O(7)	87.70(12)		
Co(2)-O(1)	2.122(2)	O(3)-Co(1)-O(10)	152.95(14)	O(6)-Co(2)-O(7)	89.94(12)		

Table S8. Weak interactions in the crystal structure of DUT-40.

Cg…Cg / X-H…Cg	Cg…Cg, Å	H…Cg, Å	X…Cg, Å	X-H..Cg, deg
Cg(1)…Cg(3)#1	4.737(2)	-	-	-
Cg(1)…Cg(3)#2	4.737(2)	-	-	-
Cg(2)…Cg(2)#1	4.868(2)	-	-	-
C(22)-H(22)…Cg(1)#1	-	2.87	3.571(4)	133
C(22)-H(22)…Cg(1)#3	-	2.87	3.571(4)	133

Symmetry operations: #1 = 1/2-X,1/2-Y,2-Z, #2 = -1/2+X,1/2-Y,-1/2+Z, #3 = 1/2+X,1/2-Y,1/2+Z
Cg1, Cg2 and Cg3 are the centers of gravity of the rings C(10)/C(11)/C(12)/C(26)/C(12)a/C(11)a, C(13)/C(14)/C(15)/C(16)/C(24)/C(25) and C(17)/C(18)/C(19)/C(20)/C(22)/C(23).

Table S9. Weak interactions in the crystal structure of DUT-41.

Cg…Cg / X-H…Cg	Cg…Cg, Å	H…Cg, Å	X…Cg, Å	X-H..Cg, deg
Cg(1)…Cg(2)#1	4.913(2)	-	-	-
Cg(3)…Cg(4)	4.7547(19)	-	-	-
Cg(3)…Cg(5)#1	4.679(2)	-	-	-
Cg(3)…Cg(6)	4.780(2)	2.87	3.571(4)	133
Cg(4)…Cg(7)#2	4.794(2)	2.87	3.571(4)	133
Cg(4)…Cg(3)	4.7545(19)	-	-	-
Cg(2)…Cg(1)#2	4.913(2)	-	-	-
Cg(2)…Cg(8)	4.916(2)	-	-	-
Cg(6)… Cg(3)	4.780(2)	-	-	-
C(10)-H(10)…Cg(4)#1	-	2.81	3.575(4)	140
C(71)-H(71)…Cg(3)#2	-	2.88	3.536(4)	129

Symmetry operations: #1 = -1/2+X,1/2-Y,-1/2+Z; #2 = 1/2+X,1/2-Y,1/2+Z
Cgx (x=1-8) are the centers of gravity of the following aromatic rings: **Cg1** C(15)/C(16)/ C(17)/ C(18)/ C(19)/C(20); **Cg2** C(62)/C(63)/C(64)/C(65)/C(73)/C(74); **Cg3** C(21)/C(22)/C(23)/C(31)/C(32)/C(45); **Cg4** C(59)/C(60)/C(61)/C(75)/C(76)/C(77); **Cg5** C(66)/C(67)/C(68)/C(69)/C(71)/C(72); **Cg6** C(78)/C(79)/C(80)/C(81)/C(82)/C(83); **Cg7** C(9)/C(10)/C(11)/C(12)/C(13)/C(14); **Cg8** C(24)/C(25)/C(26)/C(27)/C(29)/C(30)

Table S10. Weak interactions in the crystal structure of DUT-42.

Cg…Cg / X-H…Cg	Cg…Cg, Å	H…Cg, Å	X…Cg, Å	X-H..Cg, deg
Cg(1)…Cg(2)#1	4.967(2)	-	-	-
Cg(1)…Cg(2)#2	4.967(2)	-	-	-
Cg(3)…Cg(4)#1	4.8375(15)	-	-	-
Cg(3…Cg(4)#3	4.8376(15)	-	-	-
C(3)-H(3)…Cg(1)#4	-	2.96	3.825(3)	155

Symmetry operations: #1 = Y,-X+Y,1/6+Z; #2= X,X-Y,-1/6-Z; #3= X-Y,-Y,-Z; #4= X-Y,X,-1/6+Z.
Cgx (x= 1-4) are the centers of gravity of the following aromatic rings: **Cg1** C(11)/C(12)/C(13)/C(14)/C(15)/C(16); **Cg2** S(1)/C(2)/C(3)/C(3)h/C(2)h; **Cg3** C(17)/C(18)/C(19)/C(18)d/C(17)d/C(27); **Cg4** C(5)/C(6)/C(7)/C(8)/C(9)/C(10).

Table S11. Weak interactions in the crystal structure of DUT-43.

Cg…Cg / X-H…Cg	Cg…Cg, Å	H…Cg, Å	X…Cg, Å	X-H..Cg, deg
Cg(1)…Cg(2)#1	4.827(3)	-	-	-
Cg(3)…Cg(4)#2	4.680(2)	-	-	-
Cg(7)…Cg(17)#3	4.680(2)	-	-	-
Cg(5)…Cg(6)#3	4.772(3)	-	-	-
Cg(7)…Cg(8)#1	4.681(3)	-	-	-
Cg(7)…Cg(9)#	4.619(3)	-	-	-
Cg(2)…Cg(1)#	4.827(3)	-	-	-
Cg(10)…Cg(11)#4	4.736(3)	-	-	-
Cg(10)…Cg(12)#5	4.811(3)	-	-	-
Cg(13)…Cg(13)#5	4.741(3)	-	-	-
Cg(6)…Cg(5)#4	4.772(3)	-	-	-
C(134)-H(13E)…Cg(6)#6	-	2.98	3.914(10)	162
C(137)-H(13N)…Cg(14)#7	-	2.85	3.709(9)	149
C(139)-H(13P)…Cg(11)#4	-	2.95	3.814(9)	149
C(141)-H(14E)…Cg(13)	-	2.94	3.875(14)	161
C(19)-H(19)…Cg(7)#1	-	2.81	3.517(4)	134
C(44)-H(44)…Cg(10)#3	-	2.94	3.598(5)	129
C(85)-H(85)…Cg(3)#2	-	2.85	3.531(5)	131
C(85)-H(85)…Cg(3)#4	-	2.85	3.531(5)	131
C(112)-H(112)…Cg(10)#5	-	2.76	3.557(5)	145
C(126)-H(126)…Cg(7)#4	-	2.89	3.514(6)	126
C(127)-H(127)…Cg(7)#4	-	3.00	3.578(5)	122

Symmetry operations: #1 = 3/2-X,1/2-Y,2-Z; #2= 5/2-X,1/2-Y,2-Z; #3= 1/2+X,1/2-Y,1/2+Z; #4= -1/2+X,1/2-Y,-1/2+Z; #5= 1/2-X,1/2-Y,1-Z; #6= 1/2+X,1/2-Y,-1/2+Z; #7= 3/2-X,1/2-Y,1-Z

Cgx (x= 1-4) are the centers of gravity of the following aromatic rings: **Cg1** C(20)/C(21)/C(22)/C(23)/C(24)/C(25); **Cg2** C(67)/C(68)/C(69)/C(70)/C(71)/C(72); **Cg3** C(26)/C(27)/C(28)/C(27)d/C(26)d/C(37); **Cg4** C(80)/C(81)/C(82)/C(83)/C(84)/C(85); **Cg5** C(49)/C(50)/C(51)/C(52)/C(53)/C(54); **Cg6** C(117)/C(118)/C(119)/C(120)/C(128)/C(129); **Cg7** C(55)/C(56)/C(57)/C(65)/C(66)/C(73); **Cg8** C(14)/C(15)/C(16)/C(17)/C(18)/C(19); **Cg9** C(121)/C(122)/C(123)/C(124)/C(126)/C(127); **Cg10** C(99)/C(100)/C(101)/C(115)/C(116)/C(130); **Cg11** C(43)/C(44)/C(45)/C(46)/C(47)/C(48);**Cg12** C(106)/C(107)/C(108)/C(109)/C(111)/C(112); **Cg13** C(102)/C(103)/C(104)/C(105)/C(113)/C(114); **Cg14** C(2)/C(3)/C(4)/C(5)/C(6)/C(7).

Table S12. Weak interactions in the crystal structure of DUT-44.

D—H…A	D—H	H…A	D…A	D—H…A
C(3)—H(3)...O(12)#1	0.93	2.44	3.2118	140
C(18)—H(18)…O(11)#2	0.93	2.47	3.2777	145
C(48)—H(48A)…O(10)#3	0.97	2.59	3.5215	162
C(50)—H(50)…O(2)#4	0.93	2.55	3.0327	113
C(10)—H(10)…Cg(1)#5	0.93	2.86	3.4426	122
C(47)—H(47A)…Cg(2)	0.93	2.50	3.4222	160

[#1] 1/2+x,-1/2+y,z; [#2] -1/2+x,1/2-y,-1/2+z; [#3] 1/2-x,1/2+y,1/2-z; [#4] x,-y,-1/2+z; [#5] -x,1-y,-z; Cg(1) and Cg(2) are the centers of gravity of the rings C(14)/C(15)/C(16)/C(29)/C(30)/C(42) and C(21)/C(22)/C(23)/C(24)/C(25)/C(26).

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