Table S1 Crystallographic details of **Form A** and **Form B**

DATA	Form A	Form B
CCDC number	771919	771920
Formula	$C_{21}H_{26}O_4$	$C_{21}H_{26}O_4$
Formula weight	342	342
Colour	Colourless	Colourless
Crystal morphology	Block	needle
Temperature/K	293(1)	293(1)
Radiation	Mo Kα	Mo Kα
Wavelength/Å	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$P2_1$
a (Å)	8.5968(8)	10.8822(22)
b (Å)	9.7560(9)	7.4911(15)
c (Å)	23.3909(21)	12.6183(26)
α (°)	90	90
β (°)	90	110.599(3)
γ (°)	90	90
Volume (Å^3)	1961.80(3)	962.87(12)
Z	4	2
Density (g/ml)	1.16	1.18
μ (1/mm)	0.079	0.081
F (000)	735.9	368.0
θ (min, max)	1.7, 26.0	1.7, 24.7
No. Unique Refln	3845	3247
No. of parameters	232	232
R_obs, wR_2_obs	0.053, 0.107	0.034, 0.078
$\Delta\rho_{min}$, $\Delta\rho_{max}$ (eÅ^{-3})	-0.227, 0.158	-0.105, 0.118
GooF	1.150	1.058

Table S2 Intramolecular and intermolecular interactions in **Form A** and **Form B**

D–H···A	r(D–H)/Å	r(D–A)/Å	r(H···A)/Å	∠ D–H···A/º	Symmetry
Form A					
O3-H3...O4	0.820	2.741(2)	1.951(1)	161(1)	x,y,z
C11-H11...O4	0.930	3.597(3)	2.989(1)	124(1)	x,y,z
O4-H4...O3	0.820	2.844(2)	2.031(1)	171(1)	-x+2,+y-1/2,-z+1/2
C7-H7C...O4	0.960	3.348(3)	2.683(1)	126(1)	-x+2,+y+1/2,-z+1/2
C20-H20...O2	0.930	3.497(3)	2.609(1)	160(1)	x+1/2,-y+1/2,-z
C19-H19...O2	0.930	3.781(4)	2.967(2)	146(1)	x+1,+y,+z
C13-H13...O3	0.930	3.685(4)	2.808(2)	157(2)	x-1,+y,+z
Form B					
O3-H3...O4	0.820	2.659(2)	1.850(2)	168(1)	x, y, z
O4-H4...O3	0.820	2.752(2)	1.945(1)	167(1)	-x,+y+1/2,-z+1
C19-H19...O2	0.930	3.789(3)	2.988(1)	145(1)	-x,+y-1/2,-z+2
C4-H4A...Cg3[†]	0.960	3.759(3)	2.96	142(1)	x, y, z
C14-H14...Cg3[†]	0.930	3.595(3)	2.84	139(1)	1+x, y, z

[†]Cg3 is a centre of gravity of the ring formed by the atoms C16, C17, C18, C19, C20 and C21.

Table S3 Selected torsion angles (in degrees) in **Form A** and **Form B**

Torsion angle	**Form A**	**Form B**
O1-C2-C3-O2 (dioxo ring)	29.15	-24.57
C6-C2-C3-C8	-91.19	94.91
O1-C2-C6-C10	68.19	-70.20
O2-C3-C8-C16	66.01	-58.16
O1-C2-C6-O3	-169.12	168.67
O2-C3-C8-O4	-174.46	-177.14
C2-C3-C8-O4	67.91	-58.36
C2-C3-C8-C9	-177.05	-174.06

Fig. S1 PXRD patterns of **Form A** (red) and **Form B** (blue) of 2a (notice that the intensity scale (y-axis) is different in the two plots)

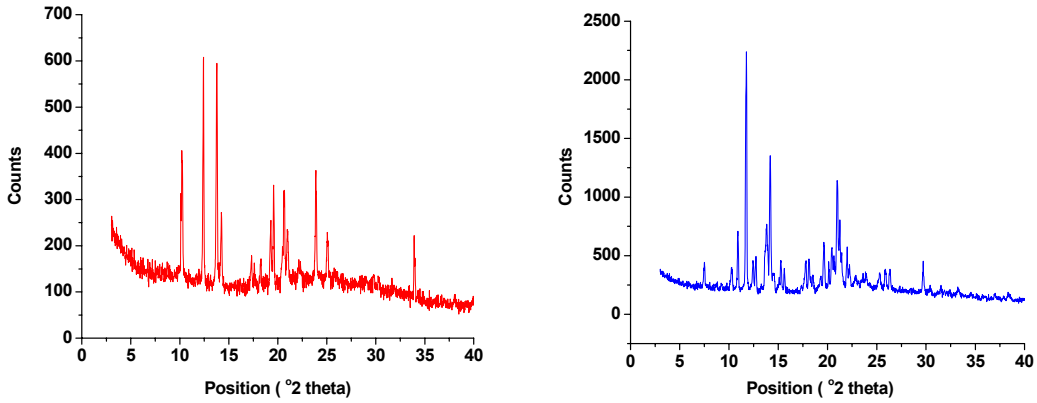

Fig. S2 IR spectra (in cm^{-1}) of **Form A** (red) and **Form B** (blue) of 2a

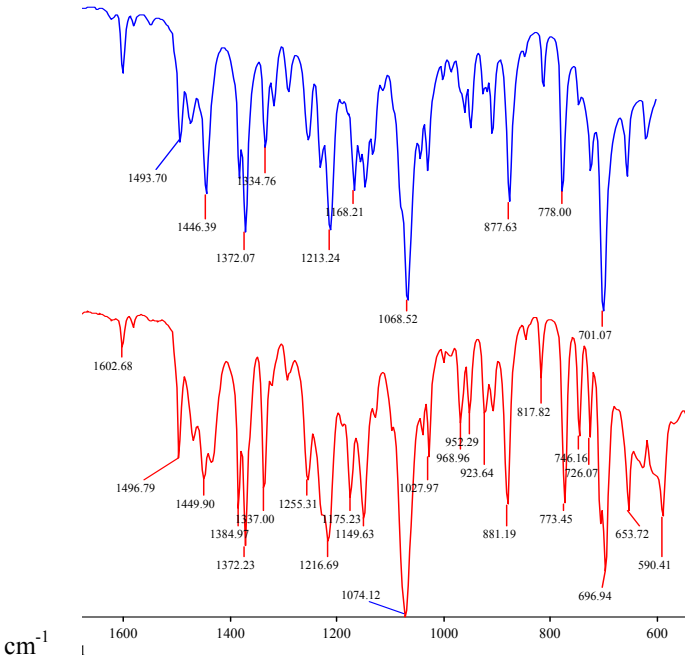

Fig. S3 Packing diagram of **Form A (**$P2_12_12_1$**)** viewed down *bc*-plane showing intra and intermolecular O-H…O interactions. The molecular dimers formed via C^{sp2}-H…O interactions are further connected via O-H…O intermolecular hydrogen bonds along the 2_1 screw in *c*-direction (Hydrogen atoms which are not involved in the hydrogen bonding are omitted for clarity).