Supplementary

S1 Crystal Structures Experimental Conditions

Table S1 Experimental details

	(izact+C6)	(izact+C7)	(izact+C8)	(izact+C9)	(izact+C10)
Chemical	$(C_2H_1N_2O)$	$\frac{2(C_{2}H_{1}N_{2}O)\cdot(C_{2})}{2(C_{2}H_{2}N_{2}O)\cdot(C_{2})}$	$\frac{(12aet + C0)}{(C + H + N + O) \cdot (C + H)}$	(C_2H_1,N_2O)	$\frac{2(C_{\rm c}H_{\rm c}N_{\rm c}O)}{2(C_{\rm c}H_{\rm c}N_{\rm c}O)}$
formula	$(C_{9}\Pi_{11}\Pi_{3}O)$	2(0,0,1)	$(C_{9}\Pi_{1}\Pi_{3}O)$ $(C_{4}$	$(C_{9}\Pi_{1}\Pi_{3}O)$	$(C_{10}H_{10}O_{10})$
M	250.28	514 58	264.3	271 32	556 66
Crystal	Monoclinic	Monoclinic $C^{2/c}$	Monoclinic	Monoclinic	Triclinic Pl
system	$P2_1/c$	wonoennie, cz/c	$P_{1/c}$	$C^{2/c}$	Thennie, 7 T
space	12110		12/10	02/0	
group					
Temperatu	173	173	173	173	173
re (K)					
a, b, c (Å)	19.0668 (10),	47.130 (4), 5.0755	19.888 (4),	22.0145 (19),	7.9554 (4),
,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	8.1886 (4),	(4), 23.567 (2)	8.2744 (15),	16.7461 (15),	13.7715 (8),
	8.0487 (4)		8.3942 (15)	7.9045 (6)	14.6005 (8)
α, β, γ (°)	90, 91.561 (3),	90, 111.352 (2),	90, 96.316 (6),	90, 100.476	72.874 (3), 75.014
	90	90	90	(3), 90	(3), 84.453 (3)
$V(Å^3)$	1256.18 (11)	5250.6 (8)	1373.0 (4)	2865.5 (4)	1476.32 (14)
Ζ	4	8	4	8	2
Radiation	Μο <i>Κ</i> α	Μο <i>Κ</i> α	Μο <i>Κ</i> α	Μο <i>Κ</i> α	Μο <i>Κ</i> α
type					
μ (mm ⁻¹)	0.10	0.10	0.09	0.09	0.09
Crystal	0.55 imes 0.20 imes	$0.46 \times 0.24 \times 0.08$	0.34 imes 0.15 imes	0.38 imes 0.20 imes	$0.36 \times 0.22 \times 0.14$
size (mm)	0.15		0.08	0.05	
F(000)	532	2192	564	1160	596
20 range	2.137 - 27.997	2.726 - 28.000	2.060 - 28.345	2.887 - 28.279	1.504 - 28.317
for data					
collection					
(°)					
Reflections	11423	50090	27737	54106	54935
collected					
Independe	$3034 [R_{int} =$	$6309 [R_{int} =$	$3282 [R_{int} =$	$3570 [R_{int} =$	7371 [$R_{int} =$
nt reflns	0.0321]	0.0389]	0.1042]	0.1327]	0.0882]
Goodness-	1.044	1.182	1.032	1.031	1.027
of-fit on					
F^2					
final R	$R_1 = 0.0465,$	$R_1 = 0.0829, wR_2$	$R_1 = 0.0664,$	$R_1 = 0.0506,$	$R_1 = 0.0528, wR_2 =$
indexes	$wR_2 = 0.1097$	= 0.1916	$wR_2 = 0.1659$	$wR_2 = 0.1077$	0.1317
$[I \ge 2\sigma(I)]$					
final R	$R_1 = 0.0701,$	$R_1 = 0.1011, wR_2$	$R_1 = 0.1118,$	$R_1 = 0.1070,$	$R_1 = 0.0783, wR_2 =$
indexes	$wR_2 = 0.1225$	= 0.1988	$wR_2 = 0.1913$	$wR_2 = 0.1354$	0.1490
[all data]					

2290718	2290719	22	90720	2290721	2290722		
ogen Bond Ta	bles						
Hydrogen-bond	geometry (Å, °) for (izact	+C6)				
		<i>D</i> —Н	$\mathrm{H}^{\dots}A$	$D \cdots A$	D—H···A		
N3 ⁱ		0.88 (2)	2.56 (2)	3.1789 (19) 128.7 (17)		
O1 ⁱ		0.88 (2)	2.65 (2)	3.515 (2)) 169.3 (18)		
··N2		0.89 (2)	1.82 (2)	2.7069 (17) 175 (2)		
Symmetry codes: (i) $x, -y+1/2, z+1/2$.							
Table S3 Hydrogen-bond geometry (Å, °) for (izact+C7)							
		<i>D</i> —Н	$\mathrm{H}^{\dots}A$	$D \cdots A$	D—H···A		
$P \cdots O1B^{i}$		0.88	2.18	3.030 (4)) 162		
····O1A ⁱ		0.88	2.16	3.016 (4)) 163		
N2 <i>A</i>		0.84	1.79	2.620 (4)) 170		
N2 <i>B</i>		0.84	1.82	2.635 (4)) 164		
code: (i) <i>x</i> , <i>y</i> –1, <i>z</i> .							
Table S4 Hydrogen-bond geometry (Å, °) for (izact+C8)							
		<i>D</i> —Н	$\mathrm{H}^{\dots}A$	$D \cdots A$	D—H···A		
··N1		0.84	1.87	2.686 (3)) 163		
Table S5 Hydrogen-bond geometry (Å, °) for (izact+C9)							
		<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H···A		
···N3 ⁱ		0.89 (3)	2.30 (3)	3.054 (2)) 142 (2)		
··O1 ⁱ		0.89 (3)	2.60 (3)	3.403 (2)) 150 (2)		
··N1		0.99 (3)	1.71 (3)	2.690 (2)) 174 (3)		
	2290718 ogen Bond Ta Hydrogen-bond N3 ⁱ O1 ⁱ \cdot N2 sodes: (i) $x, -y+1/$ Hydrogen-bond \cdots O1 A^i N2 A N2 B sode: (i) $x, y-1, z$. Hydrogen-bond \cdot N1 Hydrogen-bond \cdot N1 Hydrogen-bond	22907182290719ogen Bond TablesHydrogen-bond geometry (Å, °N3iO1i·N2codes: (i) $x, -y+1/2, z+1/2$.Hydrogen-bond geometry (Å, °····O1 B^i ····O1 A^i N2 A N2 B code: (i) $x, y-1, z$.Hydrogen-bond geometry (Å, °··N1Hydrogen-bond geometry (Å, °··N1Hydrogen-bond geometry (Å, °	2290718 2290719 22 ogen Bond Tables Hydrogen-bond geometry (Å, °) for (izact: DH N3i 0.88 (2) 0.88 (2) O1i 0.88 (2) 0.88 (2) N2 0.89 (2) 0.89 (2) codes: (i) $x, -y+1/2, z+1/2.$ Hydrogen-bond geometry (Å, °) for (izact: DH ···O1 B^i 0.88 0.84 ···O1 A^i 0.84 0.84 N2 B 0.84 0.84 N1 0.84 0.84 Hydrogen-bond geometry (Å, °) for (izact: DH ·N1 0.89 (3) 0.01 ⁱ ·N3 ⁱ 0.89 (3) 0.89 (3) ·N1 0.89 (3) 0.99 (3)	2290718 2290719 2290720 orgen Bond Tables 2290719 2290719 Hydrogen-bond geometry (Å, °) for (izact+C6) DH $H\cdots A$ N3 ⁱ 0.88 (2) 2.56 (2) O1 ⁱ 0.88 (2) 2.65 (2) $\cdot N2$ 0.89 (2) 1.82 (2) bodes: (i) x, $-y+1/2, z+1/2$. DH $H\cdots A$ Hydrogen-bond geometry (Å, °) for (izact+C7) DH $H\cdots A$ $\cdot \cdots O1A^i$ 0.88 2.18 $\cdot \cdots O1A^i$ 0.88 2.16 N2A 0.84 1.79 N2B 0.84 1.82 oode: (i) x, $y-1, z$. DH $H\cdots A$ N2B 0.84 1.87 Hydrogen-bond geometry (Å, °) for (izact+C8) DH $H\cdots A$ $\cdot N1$ 0.84 1.87 Hydrogen-bond geometry (Å, °) for (izact+C9) DH $H\cdots A$ $\cdot N1$ 0.89 (3) 2.30 (3) $\cdot O1^i$ 0.89 (3) 2.60 (3) $\cdot N1$ 0.99 (3) 1.71 (3)	2290718 2290719 2290720 2290721 ogen Bond Tables $D = H$ $H \cdots A$ $D \cdots A$ Hydrogen-bond geometry (Å, °) for (izact+C6) $D = H$ $H \cdots A$ $D \cdots A$ N3 ⁱ 0.88 (2) 2.56 (2) 3.1789 (2) O1 ⁱ 0.88 (2) 2.65 (2) 3.515 (2) ·N2 0.89 (2) 1.82 (2) 2.7069 (2) iodes: (i) x, $\neg y + 1/2$, $z + 1/2$. Hydrogen-bond geometry (Å, °) for (izact+C7) $D - H$ $H \cdots A$ Hydrogen-bond geometry (Å, °) for (izact+C7) $D - H$ $H \cdots A$ 3.016 (4) N2A 0.88 2.16 3.016 (4) N2A 0.84 1.82 2.635 (4) N2B 0.84 1.82 2.635 (4) N2B 0.84 1.82 2.686 (3) Hydrogen-bond geometry (Å, °) for (izact+C8) $D - H$ $H \cdots A$ $D \cdots A$ ·N1 0.84 1.87 2.686 (3) Hydrogen-bond geometry (Å, °) for (izact+C9) $D - H$ $D \cdots A$ ·N1 0.89 (3) 2.30 (3)		

Symmetry codes: (i) x, -y+1, z+1/2.

Table S6 Hydrogen-bond geometry (Å, °) for (izact+C10)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H···A
N2—H2 B ····N6 ⁱ	0.88 (2)	2.35 (2)	3.088 (2)	141.8 (18)
N2—H2 B ····O6 ⁱ	0.88 (2)	2.60 (2)	3.384 (2)	149.2 (17)
O2—H2…N1	0.96 (3)	1.80 (3)	2.706 (2)	156 (3)
O4—H4…N4	0.94 (3)	1.74 (3)	2.6770 (18)	176 (3)
N5—H5A····N3 ⁱⁱ	0.84 (2)	2.31 (2)	3.0476 (19)	147.4 (19)

Symmetry codes: (i) -x+1, -y+1, -z+1; (ii) -x+2, -y+1, -z+1.

S2 PXRD Patterns



Figure S1 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C6, together with the calculated patterns of its coformers in their pure form.



Figure S2 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C7, together with the calculated patterns of its coformers in their pure form.



Figure S3 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C8, together with the calculated patterns of its coformers in their pure form.



Figure S4 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C9, together with the calculated patterns of its coformers in their pure form.



Figure S5 Powder patterns for the experimental and calculated patterns of the cocrystal of izact + C7, together with the calculated patterns of its coformers in their pure form.



S3 DSC Analysis

Figure S6 DSC curve of izact + C6







Figure S8 DSC curve of izact + C8



Figure S9 DSC curve of izact + C9



Figure S10 DSC curve of izact + C10





Figure S11 FTIR Spectra of izact + C6.



Figure S12 FTIR Spectra of izact + C7.



Figure S13 FTIR Spectra of izact + C8.



Figure S14 FTIR Spectra of izact + C9.



Figure S15 FTIR Spectra of izact + C10.

Table S7 Some FTIR assignments for	the cocrystals of izact with	dicarboxylic
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acids.

Solid form	v (-C=O)	ν(-NH-)	v (-OH)
izact + C6	1697.19	3196.66	2941.77
izact + C7	1633.75	3267.29	2944.95
izact + C8	1709.44	3307.85	2946.19
izact + C9	1670.66	3222.19	2945.48
izact + C10	1668.81	3231.23	2937.37