Electronic Supplementary Material (ESI) for Chemical Communications

Supplementary Information

Structural Landscape of the Benzoic Acid:Isonicotinamide 1:1 Cocrystal

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G-1: Data collection and refinement details, crystallization methods

- Single crystal X-ray diffraction

Single crystal X-ray data for 246TFBA:INAwere collected on an Bruker Kappa Apex II CCD diffractometer using Mo-KΣ[1](λ= 0.71073 Å). The crystal was maintained at the desired temperature during data collection using Oxford cryosystems N_2open flow cryostat[2]. The remaining crystal data were collected on a Rigaku Mercury375R/M CCD (XtaLAB mini) diffractometer using graphite monochromated Mo-Kα radiation, equipped with a Rigaku low temperature gas spray cooler, data were processed with the RigakuCrystalClear software[3]. Structure solution and refinement were performed using SHELX-2013[4]embedded in the WinGX suite[5] and Olex2.[6]Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms for all structures were located on the difference Fourier map.The hydrogen bond tableswere created using PLATON.[7] Mercury version 3.0 was used for molecular representations and packing diagrams.[8]

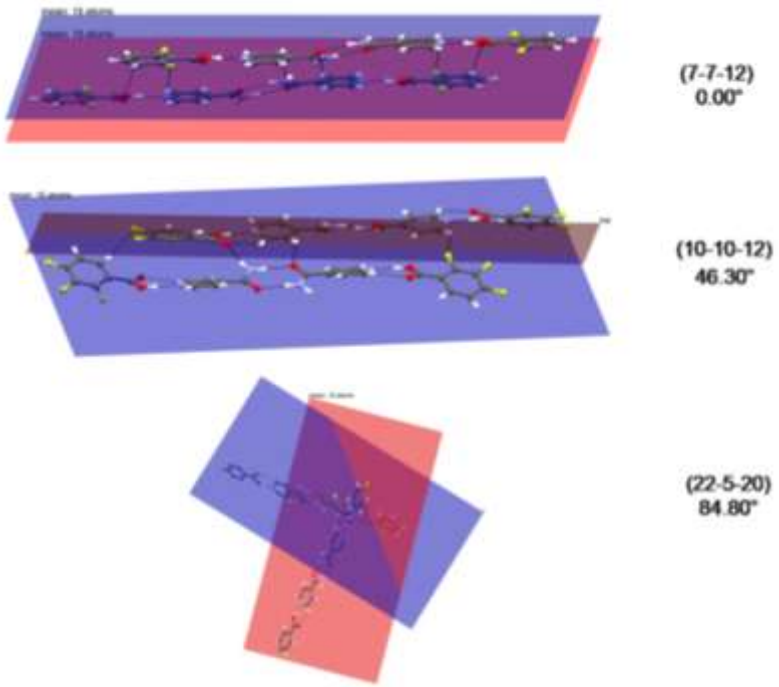
1. Bruker APEX2 (Version 1.0.22), BIS (Version 1.2.08), COSMO (Version 1.48) and SAINT(Version 7.06A), Bruker AXS Inc., Madison, Wisconsin, USA. 2006.
2. Oxford Instruments, Cryojet XL/HT controller; Oxford Diffraction Ltd.: Yarnton, England.
3. CrystalClear 2.0, Rigaku Corporation, Tokyo, Japan.
4. G. M. Sheldrick, *ActaCrystallogr., Sect. A*, 2008, **64**, 112.
5. L. J. Farrugia, *J. Appl. Crystallogr.* 1999, **32**, 837.
6. O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, .*J. Appl. Crystallogr.*, 2009, **42**, 339.
7. A. L. Spek, *J. Appl. Crystallogr.*, 2003, **36**, 7.
8. C. F. Macrae, P. R. Edgington, P. McCabe, E.Pidcock, G. P.Shields, R.Taylor, M.Towler, J.van de Streek, *J. Appl. Crystallogr.*, 2006, **39**, 453.

- Crystallization Methods

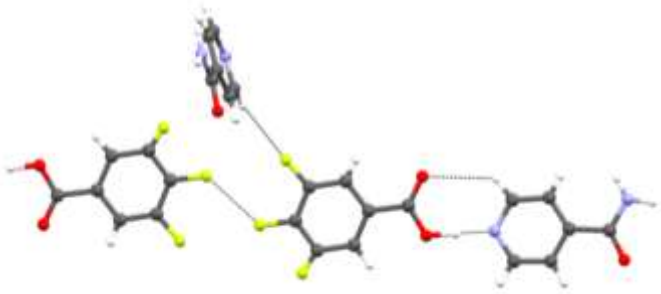
All compoundswere purchased from Sigma-Aldrich and Alfa-Aesar, and were used without further purification.

All crystallization experiments were carried out at ambient conditions. In order to get good quality single crystals for X-ray diffraction, we used several crystallization methods; solvent evaporation, anti-solvent, vapor-diffusion, with various stoichiometric ratios. In the solvent evaporation method,crystals were obtained within three to four days while in the vapor-diffusion method, crystalswere obtained after two weeks.

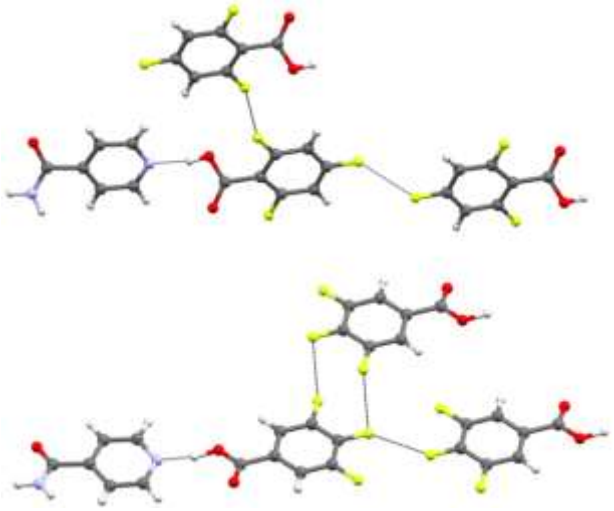
R-1: Diagrams of experimental crystal structures



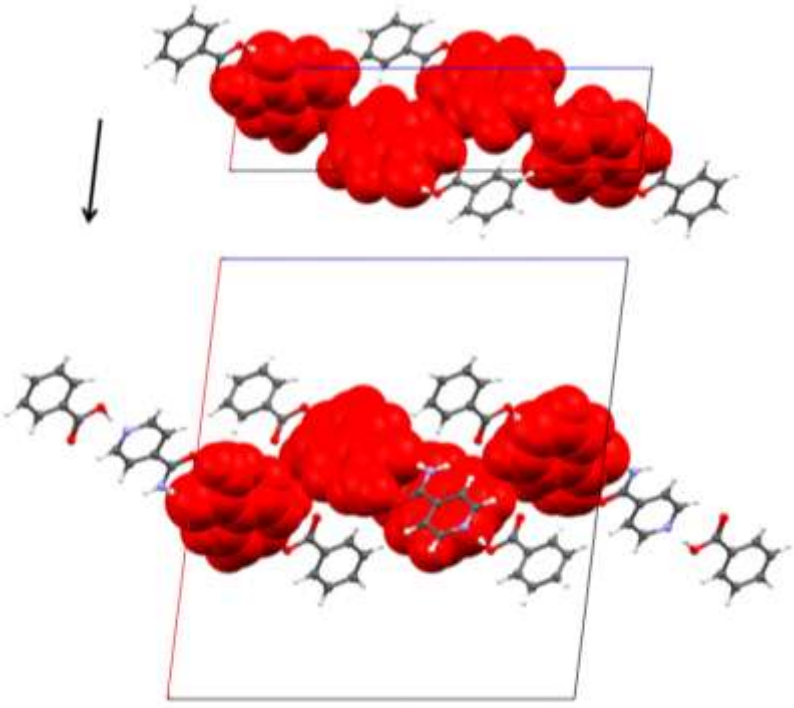
(a). Structure types in the 1:1 BA:INA structural landscape. Red and blue color coding refers to molecular planes that contain fluorobenzoic acids. The angles between the planes are indicated.



(b). Nature of F···F interaction in 34DFBA:INA, the blueprint of 3FBA:INA as well as 4FBA:INA cocrystals

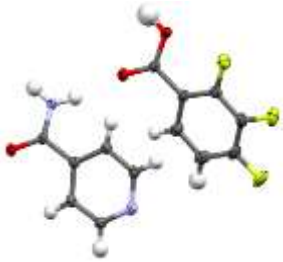
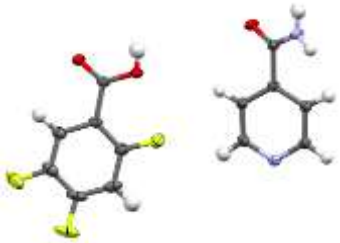
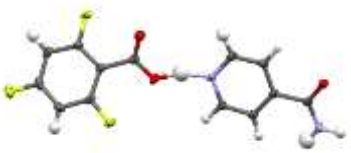
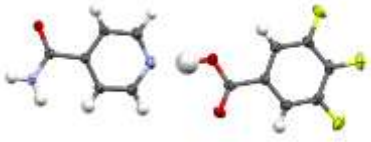
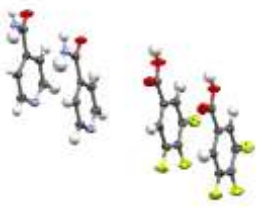


(c).246TFBA:INA (above) and 345TFBA:INA (below) crystal structures.
These two crystal structures are distinguishable based on the role of the F···F synthons.



(d).BA (above) and BA:INA (below) crystal structures, *ac* plane.
Arrow shows the four time extension along a-axis.

R-2: ORTEP diagrams for the asymmetric unit of the crystal structures (ellipsoids are drawn at 50% probability). Disordered structures are indicated with an asterix. Only the asymmetric unit is shown.

		
2,4-Difluorobenzoic acid:Isonicotinamide	2,5-Difluorobenzoic acid:Isonicotinamide	2,6-Difluorobenzoic acid:Isonicotinamide
		
3,4-Difluorobenzoic acid:Isonicotinamide	3,5-Difluorobenzoic acid:Isonicotinamide	3,5-Difluorobenzoic acid:Isonicotinamide Hydrate
		
2,3,4-Trifluorobenzoic acid:Isonicotinamide	2,4,5-Trifluorobenzoic acid:Isonicotinamide	2,4,6-Trifluorobenzoic acid:Isonicotinamide-I
		
2,4,6-Trifluorobenzoic acid:Isonicotinamide-II	3,4,5-Trifluorobenzoic acid:Isonicotinamide-I	3,4,5-Trifluorobenzoic acid:Isonicotinamide-II

2,3,4,5-Tetrafluorobenzoic acid:Isonicotinamide

2,3,4,5,6-Pentafluorobenzoic acid:Isonicotinamide

D-1: Normalized hydrogen bond distances for the compounds in this study

Compound	D–H···A[#]	r(D–H)/Å	r(D–A)/Å	r(H···A)/Å	∠ D–H···A/°	Symmetry
24DFBA:INA	N(1)–H(1A)...O(1)	1.01	3.0050(18)	2.02	163	-x,1-y,1-z
	N(1)–H(1B)...F(1)	1.01	2.8965(18)	2.51	102	-x,1-y,1-z
	N(1)–H(1B)...O(3)	1.01	2.9116(17)	1.92	167	-x,1-y,1-z
	O(2)–H(2)...N(2)	0.98	2.5910(17)	1.62	170	x,1+y,-1+z
	C(6)–H(6)...O(1)	1.08	3.350(2)	2.52	133	x,-1+y,z
	C(11)–H(11)...O(3)	1.08	3.4243(19)	2.47	146	-x,-y,1-z
25DFBA:INA	O(1)–H(1)...N(1)	0.98	2.628(2)	1.65	176	
	N(2)–H(2A)...O(3)	1.01	2.942(2)	1.93	177	2-x,1-y,1-z
	N(2)–H(2B)...F(3A)	1.01	3.017(2)	2.47	113	1-x,1-y,1-z
	N(2)–H(2B)...O(5)	1.01	3.078(2)	2.08	168	1-x,1-y,1-z
	N(4)–H(4A)...O(6)	1.01	2.879(2)	1.88	173	1-x,-y,2-z
	N(4)–H(4B)...O(2)	1.01	2.879(2)	1.89	165	x,-1+y,z
	O(4)–H(4O)...N(3) intra	0.98	2.550(2)	1.57	175	-x,1-y,1-z
	C(2)–H(2)...F(4A)	1.08	3.255(3)	2.39	136	-1+x,-1+y,z
	C(4)–H(4)...F(2)	1.08	3.453(3)	2.37	176	-1-x,1-y,2-z
	C(5)–H(5)...O(6)	1.08	3.348(3)	2.29	164	-x,1-y,2-z
	C(8)–H(8)...F(3A)	1.08	3.085(3)	2.44	117	
	C(8)–H(8)...O(2)	1.08	3.153(3)	2.36	128	
	C(11)–H(11)...O(5)	1.08	3.355(3)	2.29	168	1-x,1-y,1-z
	C(12)–H(12)...O(4)	1.08	3.252(3)	2.34	140	x,-1+y,z
	C(24)–H(24)...O(2)	1.08	3.383(3)	2.34	161	x,-1+y,z
	C(25)–H(25)...O(3)	1.08	3.252(3)	2.45	130	-1+x,-1+y,z
26DFBA:INA	O(1)–H(1)...N(1)	0.98	2.5650(14)	1.59	170	x,-1+y,1+z
	N(2)–H(2A)...O(3)	1.01	2.8904(15)	1.89	168	1-x,-y,1-z
	N(2)–H(2B)...O(2)	1.01	2.9450(14)	1.95	167	1-x,-y,1-z
	C(13)–H(13)...F(1)	1.08	3.0156(16)	2.26	125	x,y,-1+z
34DFBA:INA	O(2)–H(2)...N(1)	0.98	2.569(2)	1.59	179	-x,-1+y,1/2-z

	N(2)–H(2A)...O(3)	1.01	2.877(2)	1.87	173	-x,1-y,-z
	N(2)–H(2B)...O(1)	1.01	2.945(2)	1.95	170	-
	C(6)–H(6)...O(1)	1.08	3.352(3)	2.33	156	-
35DFBA:INA	O(1)–H(1)...N(1)	0.98	2.586(4)	1.62	167	1-x,-y,1-z
	N(2)–H(2A)...O(2)	1.01	2.923(5)	1.98	154	-
	N(2)–H(2B)...O(3)	1.01	2.860(5)	1.85	179	3-x,1-y,1-z
	C(11)–H(11)...F(1)	1.08	3.318(5)	2.32	153	x,-1+y,1+z
35DFBA:INA hydrate	O(2)–H(2)...N(1)	0.98	2.566(3)	1.59	173	1+x,1-y,1/2+z
	N(2)–H(2B)...O(4)	1.01	2.900(3)	1.95	157	x,-1+y,z
	N(2)–H(2C)...O(1)	1.01	2.911(3)	2.06	141	x,-1+y,z
	O(4)–H(4A)...O(3)	0.98	2.807(3)	1.86	160	-1+x,1-y,-1/2+z
	O(4)–H(4B)...O(1)	0.98	2.967(3)	2.01	164	-1+x,y,z
	C(2)–H(2A)...O(3)	1.08	3.302(3)	2.35	146	x,-y,-1/2+z
	C(4)–H(4)...F(2)	1.08	3.229(3)	2.38	134	-1+x,y,z
	C(4)–H(4)...F(1)	1.08	3.389(3)	2.48	141	x,1-y,1/2+z
	C(6)–H(6)...O(1)	1.08	3.219(3)	2.38	133	-1+x,1-y,-1/2+z
	C(8)–H(8)...O(4)	1.08	3.465(3)	2.46	153	-
234TFBA:INA	O(2)–H(2)...N(1)	0.98	2.6206(16)	1.64	174	x,3/2-y,-1/2+z
	N(2)–H(2A)...O(1)	1.01	2.8714(17)	1.89	165	-
	N(2)–H(2B)...O(3)	1.01	2.9415(16)	1.93	176	1-x,1-y,-z
	C(3)–H(3)...O(3)	1.08	3.2737(19)	2.39	137	1-x,1/2+y,1/2-z
	C(5)–H(5)...O(1)	1.08	3.1148(18)	2.34	127	x,3/2-y,1/2+z
	C(8)–H(8)...F(3)	1.08	3.164(2)	2.46	121	x,3/2-y,-1/2+z
245TFBA:INA	O(1)–H(1)...N(1)	0.98	2.6031(17)	1.62	178	x,1/2-y,1/2+z
	N(2)–H(2A)...O(2)	1.01	2.8762(19)	1.88	167	x,-1+y,z
	N(2)–H(2B)...O(3)	1.01	2.9471(18)	1.94	175	2-x,-y,2-z
	C(4)–H(4)...O(3)	1.08	3.212(2)	2.36	135	2-x,-1/2+y,3/2-z
	C(6)–H(6)...O(2)	1.08	3.1173(19)	2.35	127	x,1/2-y,-1/2+z
	C(9)–H(9)...F(1)	1.08	3.146(2)	2.38	126	
	C(13)–H(13)...F(3)	1.08	3.429(2)	2.39	160	1-x,-1/2+y,1/2-z
246TFBA:INA(I)	O(2)–H(2)...N(1)	0.98	2.500(2)	1.55	162	2-x,-y,-z
	N(2)–H(2A)...O(3)	1.01	2.896(2)	1.89	177	1-x,1-y,-z
	N(2)–H(2B)...O(2)	1.01	2.982(2)	1.98	169	1-x,1-y,-z
	C(8)–H(8)...F(1)	1.08	3.150(3)	2.32	132	2-x,1-y,-z
	C(9)–H(9)...O(2)	1.08	3.201(3)	2.19	154	1-x,1-y,-z
246TFBA:INA(II)	O(1)–H(1)...N(1)	0.98	2.500(2)	1.55	162	2-x,-y,-z
	N(2)–H(2A)...O(3)	1.01	2.896(2)	1.89	177	1-x,1-y,-z
	N(2)–H(2B)...O(2)	1.01	2.982(2)	1.98	169	1-x,1-y,-z
	C(8)–H(8)...F(1)	1.08	3.150(3)	2.32	132	2-x,1-y,-z
	C(9)–H(9)...O(2)	1.08	3.201(3)	2.19	154	2-x,1-y,-z
345TFBA:INA(I)	O(1)–H(1)...N(1)	0.98	2.594(3)	1.62	170	-

	N(2)–H(2A)...O(2)	1.01	2.945(3)	1.98	158	1-x,1-y,1-z
	N(2)–H(2B)...O(3)	1.01	2.855(3)	1.85	174	-1-x,2-y,1-z
	C(10)–H(10)...F(1)	1.08	3.327(3)	2.39	144	1-x,-y,2-z
	C(11)–H(11)...F(3)	1.08	3.364(3)	2.43	144	-2+x,1+y,z
345TFBA:INA(II)	O(4)–H(1)...N(3)	0.98	2.580(5)	1.63	162	1+x,y,z
	O(2)–H(2)...N(1)	0.98	2.586(4)	1.63	163	1+x,y,z
	N(4)–H(3)...O(5)	1.01	2.871(5)	1.86	176	-x,-1-y,1-z
	N(4–H(4)...O(1)	1.01	2.962(5)	1.99	160	-x,-y,1-z
	N(2)–H(9)...O(6)	1.01	2.849(5)	1.84	175	-x,-1-y,1-z
	N(2)–H(10)...O(3)	1.01	2.930(5)	2.14	134	-x,-y,1-z
	C(25)–H(8)...F(1)	1.08	3.283(5)	2.45	133	-x,-y,2-z
	C(19)–H(14)...F(4)	1.08	3.340(5)	2.34	153	-x,-y,2-z
2345TeFBA:INA	O(1)–H(1)...N(1)	0.98	2.5980(17)	1.62	179	x,-1+y,-1+z
	N(2)–H(2A)...O(2)	1.01	2.8477(19)	1.86	165	x,3/2-y,1/2+z
	N(2)–H(2B)...O(3)	1.01	2.9643(18)	1.96	176	-x,2-y,-z
	C(8)–H(8)...O(3)	1.08	3.251(2)	2.40	135	-x,1/2+y,1/2-z
	C(11)–H(11)...O(2)	1.08	3.0700(19)	2.26	130	x,1+y,1+z
	C(13)–H(13)...F(1)	1.08	3.271(2)	2.47	130	x,1/2-y,1/2+z
23456PFBA:INA	N(1)–H(1)...O(2)	1.01	2.602(2)	1.60	174	1-x,1/2+y,1/2-z
	N(1)–H(1)...O(3)	1.01	3.192(3)	2.58	119	1-x,1/2+y,1/2-z
	N(2)–H(2A)...O(1)	1.01	2.964(3)	1.97	170	2-x,2-y,2-z
	N(2)–H(2B)...O(3)	1.01	2.783(3)	1.85	152	1-x,2-y,1-z
	C(6)–H(6)...O(3)	1.08	3.051(3)	2.26	128	1-x,1/2+y,1/2-z
	C(13)–H(13)...F(5)	1.08	3.095(3)	2.37	123	1-x,1-y,1-z

D-2: Crystallographic tables of the experimental structures

Compound	**24DFBA:INA**	**25DFBA:INA**	**26DFBA:INA**	**34DFBA:INA**	**35DFBA:INA**
CCDC No.	965666	965667	965668	965671	965673
Molecular formula	$C_7H_3F_2O_2$, $C_6H_6N_2O$	$C_{14}H_8F_4O_4$, $C_{12}H_{12}N_4O_2$	$C_7H_4F_2O_2$, $C_6H_6N_2O$	$C_7H_3F_2O_2$, $C_6H_6N_2O$	$C_7H_4F_2O_2$, $C_6H_6N_2O$
Formula weight	279.22	1116.89	280.23	279.22	280.23
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Triclinic
Space group	*P*1	*P*1	*P*1	*C*2/c	*P*1
***a* (Å)**	7.0231(8)	8.3252(6)	7.2755(7)	22.920(4)	6.57(1)
***b* (Å)**	7.4789(9)	12.1896 (9)	7.6883 (8)	5.2259 (8)	7.680 (11)
***c* (Å)**	12.6456(15)	13.477(1)	12.5950(13)	20.566(3)	13.084(18)
***α* (°)**	74.419(5)	107.408(8)	73.583(5)	90	92.357(15)
***β* (°)**	87.775(6)	102.834(7)	84.326(6)	97.914(12)	90.759(9)
***γ* (°)**	70.545(5)	94.816(7)	66.372(5)	90	109.87(3)
***V* (Å^3)**	602.33(13)	1255.68(18)	619.06(11)	2439.9(7)	620.1(16)

ρcalc (g/cm^3)	1.540	1.477	1.503	1.520	1.501
F(000)	286.0	572	288	1144	288
μ (mm^{-1})	0.131	0.126	0.128	0.129	0.128
T (K)	150K	150K	150K	150K	150K
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Reflns. collected	6013	13487	6605	11631	6419
Unique reflns.	2762	5746	2839	2794	2808
Completeness (%)	99.7	99.8	99.8	99.8	98.7
R_{int}	0.023	0.032	0.014	0.040	0.069
R_1 (F^2)	0.044	0.0501	0.0356	0.0533	0.0440
wR_2(F^2)	0.117	0.1395	0.1061	0.1291	0.1353
Goodness-of-fit	1.05	1.05	1.074	1.026	1.081
Resolution (*2θ*)	54	54	54	54	54

Compound	**35DFBA:INA hydrate**	**234TFBA:INA**	**245TFBA:INA**	**246TFBA:INA(I)**	**246TFBA:INA (II)**
CCDC No.	965672	965662	965663	965664	965665
Molecular formula	$C_7H_4F_2O_2$, $C_6H_6N_2O$, H_2O	$C_7H_3F_3O_2$, $C_6H_6N_2O$	$C_7H_3F_3O_2$, $C_6H_6N_2O$	$C_7H_3F_3O_2$, $C_6H_6N_2O$	$C_{14}H_6F_6O_4$, $C_{12}H_{12}N_4O_2$
Formula weight	298.25	298.22	298.22	298.22	596.44
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	*P*c	*P*2$_1$/c	*P*2$_1$/c	*P*1	*P*1
a (Å)	3.7357(5)	10.1728(12)	10.4383(9)	7.2331(14)	3.8198(6)
b (Å)	15.625 (2)	10.4501(13)	10.2939(9)	7.7199(15)	7.5011(9)
c (Å)	10.9260(14)	12.2561(15)	12.3077(10)	12.597(2)	21.814(3)
α (˚)	90	90	90	73.687(5)	98.435(8)
β (˚)	93.614(7)	109.116(8)	110.475(8)	84.340(6)	93.169(8)
γ (˚)	90	90	90	66.993(5)	97.474(7)
V (Å^3)	636.49(14)	1231.1(3)	1238.93(19)	621.3(2)	611.25(15)
ρcalc (g/cm^3)	1.556	1.609	1.599	1.594	1.620
F(000)	308	608	608	304	304
μ. (mm^{-1})	0.135	0.145	0.144	0.144	0.146
T (K)	150K	150K	150K	150K	100K
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Reflns. collected	6570	12048	12810	6167	7504
Unique reflns.	1465	2808	2823	2832	2662
Completeness (%)	99.8	99.9	99.9	99.3	99.8
R_{int}	0.031	0.026	0.038	0.034	0.039
R_1 (F^2)	0.0307	0.0393	0.0424	0.0474	0.0487
wR_2(F^2)	0.0752	0.1011	0.1066	0.1216	0.1288
Goodness-of-fit	1.08	1.048	1.045	1.037	0.96
Resolution (2θ)	54	54	54	54	54

Compound	345TFBA:INA(I)	345TFBA:INA(II)	2345TeFBA:INA	23456PFBA:INA
CCDC No.	965669	965670	965661	965660
Molecular formula	$C_7H_3F_3O_2$, $C_6H_6N_2O$	$C_7H_3F_3O_2$, $C_6H_6N_2O$	$C_7H_1F_4O_2$, $C_6H_6N_2O$	$C_7F_5O_2$, $C_6H_7N_2O$
Formula weight	298.22	298.22	315.21	334.20
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	*P*1	*P*1	$P2_1/c$	$P2_1/c$
a (Å)	6.8789(12)	7.7191(14)	10.1699(7)	10.421 (4)
b (Å)	7.2488 (13)	10.869 (2)	10.3825(7)	10.421(3)
c (Å)	13.638(3)	15.312(3)	12.3583(9)	12.704(3)
α (˚)	89.962(6)	73.545(5)	90	90
β (˚)	81.279(7)	86.948(6)	108.977(8)	114.190(9)
γ (˚)	66.888(8)	85.853(6)	90	90
V ($Å^3$)	616.9(2)	1228.1(4)	1233.98(16)	1258.5(11)
ρcalc (g/cm^3)	1.605	1.613	1.697	1.764
F(000)	304	608	636	672
μ. (mm^{-1})	0.145	0.145	0.161	0.174
T (K)	150K	150K	150K	150K
λ (Å)	0.71073	0.71073	0.71073	0.71073
Reflns. collected	6576	12973	12858	11390
Unique reflns.	2820	5593	2822	2888
Completeness (%)	100	99.7	99.9	99.7
R_{int}	0.036	0.090	0.033	0.062
R_1 (F^2)	0.0488	0.0720	0.0400	0.0485
wR_2(F^2)	0.1294	0.1993	0.1062	0.1315
Goodness-of-fit	1.072	0.985	1.072	1.021
Resolution (2θ)	54	54	54	54

D-3: Computational details for ESP charge calculations and Polymorph prediction protocols for 1:1 BA:INA cocrystal

Cell parameters of predicted structures	
18^{th} Rank	6^{th} Rank
*C*2/c, v=2492.87	*P*1, V=610.767
a=22.0625, α=90	a=7.8227, α=77.6135
b=5.3206, β=83.9480	b=7.0629, β=112.9878
c=21.3556, γ=90	c=13.0459, γ=112.6180

For ESP charge calculation

```
==================================================
                  DMol3 Run Status
==================================================

Job Name            :        2FBA_OPT
Task                :        Property
Basis               :        dnp
Atom_Rcut           :        3.700 Angstrom
Functional          :        pbe
Harris              :        off
Integration Grid    :        fine
Occupation          :        fermi
Pseudopotential     :        none
Property            :        Plot Data

==================================================

# Task parameters
Calculate                      optimize
Opt_energy_convergence         1.0000e-005
Opt_gradient_convergence       2.0000e-003 A
Opt_displacement_convergence   5.0000e-003 A
Opt_iterations                 50
Opt_max_displacement           0.3000 A
Initial_hessian                improved
Symmetry                       on
Max_memory                     2048

# Electronic parameters
Spin_polarization              restricted
Charge                         0
Basis                          dnp
Pseudopotential                none
Functional                     pbe
Aux_densityoctupole
Integration_grid               fine
Occupation                     fermi
Cutoff_Global                  3.7000 angstrom
Scf_density_convergence        1.0000e-006
Scf_charge_mixing              0.2000
Scf_iterations                 50
Scf_diis                       6 pulay

# Print options
Print                          eigval_last_it

# Calculated properties
Plot                           potential
Mulliken_analysis              charge
Hirshfeld_analysis             charge
Esp_fit                        on
Grid                           msbox  3 0.2500 0.2500 0.2500 3.0000

====================================
```

```
Summary of ESP fitting calculations
Number of points         :     144490
Total integration weight :   40599.34
Spacing between          :       0.25 Ang
Sigma                    : 0.1731E-02
RMS of V(exact)          : 0.1680E-01
RRMS fit                 :      10.30 %

ESP-fitted charges        :
nElem    chgvdW(in)  vdW(ex)
    1  H      0.166   1.30   2.80
    2  O     -0.549   1.72   3.22
    3  O     -0.477   1.72   3.22
    4  C      0.143   2.00   3.50
    5  C     -0.208   2.00   3.50
    6  C     -0.062   2.00   3.50
    7  C     -0.163   2.00   3.50
    8  C     -0.097   2.00   3.50
    9  C     -0.219   2.00   3.50
   10  C      0.478   2.00   3.50
   11  H      0.166   1.30   2.80
   12  O     -0.448   1.72   3.22
   13  N     -0.632   1.83   3.33
   14  N     -0.778   1.83   3.33
   15  C      0.470   2.00   3.50
   16  C     -0.558   2.00   3.50
   17  C      0.419   2.00   3.50
   18  C     -0.555   2.00   3.50
   19  C      0.437   2.00   3.50
   20  C      0.438   2.00   3.50
   21  H      0.421   1.30   2.80
   22  H      0.136   1.30   2.80
   23  H      0.130   1.30   2.80
   24  H      0.122   1.30   2.80
   25  H      0.396   1.30   2.80
   26  H      0.347   1.30   2.80
   27  H      0.035   1.30   2.80
   28  H      0.198   1.30   2.80
   29  H      0.198   1.30   2.80
   30  H      0.043   1.30   2.80
```

ForPolymorph Prediction protocols

```
              Polymorph

Mode              : New calculation
Protocol          : Packing >> Clustering >> Geometry Optimization >>
Clustering
Version           : 6.0
Build date        : Dec  8 2011
Host              : ritesh
Operating system  : Windows
Task started      : Wed Sep 04 09:33:00 2013
```

```
---- Packing parameters ----

Search algorithm                : MC Simulated Annealing
Maximum number of steps         : 7000
Explore torsions                : No
Preoptimize structures          : No
Steps to accept before cooling  : 12
Minimum move factor             : 0.1000E-08
Heating factor                  : 0.02500
Maximum temperature             : 100000.0 K
Minimum temperature             : 300.0 K


---- Cluster analysis parameters ----

Cluster grouping                : Forcefield type
Cutoff                          : 7.000
Number of bins                  : 140
Tolerance                       : 0.1300
Maximum number of clusters      : All clusters

---- Geometry optimization parameters ----

Algorithm                       : Smart
Convergence tolerance:
  Energy                        : 0.0001 kcal/mol
  Force                         : 0.005 kcal/mol/A
  Stress                        : 0.005 GPa
  Displacement                  : 5e-005 A
Maximum number of iterations    : 500
External pressure               : 0 GPa
Motion groups rigid             : NO
Optimize cell                   : YES


---- Energy parameters ----

Forcefield                      : Dreiding
Electrostatic terms:
  Summation method              : Ewald
  Accuracy                      : 0.0001 kcal/mol
  Buffer width                  : 0.5 A

van der Waals terms:
  Summation method              : Ewald
  Accuracy                      : 0.0001 kcal/mol
  Repulsive cutoff              : 6 A
  Buffer width                  : 0.5 A

Hydrogen bond terms:
  Summation method              : Atom based
  Truncation method             : Cubic spline
  Cutoff distance               : 4.5 A
  Spline width                  : 0.5 A
  Buffer width                  : 0.5 A
```

```
#####################################
Processing space group : P21/C
#####################################

---- Packing ----

Space group                     : P 1 21/C 1
Random number seed              : 98228021
Cooling factor                  : 0.00100
Number of trials made           : 5933
Number of trials saved          : 3714 (62.6%)
Maximum temperature achieved    : 11454.7 K
Final temperature               : 299.9 K

---- Cluster analysis ----

Lowest energy clusters (20 maximum):

Cluster   Frame   Cluster size  Energy (kcal/mol/asym. cell)
    1     3277          3       2.831
    2     3278          2       2.846
    3     3227          1       3.078
    4     3228          9       3.155
    5     3257          5       3.302
    6     3273          1       3.404
    7     3294          1       3.418
    8     3261          6       3.474
    9     3292          1       3.494
   10     3314         10       3.540
   11     3291          1       3.575
   12     3289          1       3.586
   13     3239          1       3.620
   14     3300          2       3.633
   15     3285          2       3.665
   16     3328          1       3.696
   17     3296          2       3.709
   18     3226          1       3.728
   19     3329         14       3.748
   20     3295          1       3.773


Calculation summary:

Number of frames searched           : 3714
Number of clusters found            : 3154
Number of frames put into a cluster : 3714 (100 %).

---- Geometry optimization ----

Total number of frames        : 3154
Frames with lowest energy:
  Order   Frame     Energy (kcal/mol/asym. cell)
    1     1217              -69.595
    2      923              -69.595
    3     2183              -69.595
```

4	2147	-69.595
5	1611	-69.595
6	1294	-69.595
7	1485	-69.595
8	3050	-69.595
9	325	-69.595
10	1067	-69.595
11	1258	-69.595
12	1682	-69.592
13	1296	-69.592
14	1956	-69.592
15	1814	-69.585
16	1667	-69.584
17	293	-69.255
18	283	-69.255
19	219	-69.255
20	189	-69.255

---- Cluster analysis ----

Lowest energy clusters (20 maximum):

Cluster	Frame	Cluster size	Energy (kcal/mol/asym. cell)
1	1217	11	-69.595
2	1682	3	-69.592
3	1814	1	-69.585
4	1667	1	-69.584
5	293	121	-69.255
6	647	2	-69.073
7	2330	1	-69.068
8	2760	3	-68.943
9	676	4	-68.909
10	1782	3	-68.865
11	2103	5	-68.864
12	363	4	-68.791
13	1335	3	-68.780
14	1787	1	-68.702
15	673	5	-68.581
16	1447	2	-68.530
17	1649	9	-68.514
18	2955	1	-68.507
19	2378	1	-68.475
20	2634	1	-68.377

Calculation summary:

Number of frames searched : 3154
Number of clusters found : 1697
Number of frames put into a cluster : 3154 (100 %).

##
Processing space group : P-1
##

---- Packing ----

Space group : P -1

```
Random number seed              : 207600621
Cooling factor                  : 0.00100
Number of trials made           : 4682
Number of trials saved          : 2569 (54.9%)
Maximum temperature achieved    : 3770.6 K
Final temperature               : 300.0 K


---- Cluster analysis ----

Lowest energy clusters (20 maximum):

Cluster   Frame   Cluster size  Energy (kcal/mol/asym. cell)
    1     1338          1       4.028
    2      280          1       4.057
    3      982          1       4.903
    4      977          1       4.920
    5      727          1       5.042
    6     1000          3       5.292
    7     1339          1       5.303
    8      730          1       5.422
    9     1087          1       5.583
   10      985          2       5.602
   11     1335          1       5.705
   12     2065          2       5.751
   13      728          1       5.805
   14     2069          8       5.821
   15     2168         17       5.886
   16      989          8       5.891
   17     1135          1       5.910
   18     2066          1       5.955
   19     2164          9       5.992
   20     1668          1       6.042


Calculation summary:

Number of frames searched           : 2569
Number of clusters found            : 2018
Number of frames put into a cluster : 2569 (100 %).


---- Geometry optimization ----

Total number of frames        : 2018
Frames with lowest energy:
  Order   Frame     Energy (kcal/mol/asym. cell)
    1      165              -70.584
    2      700              -70.584
    3      973              -70.584
    4      703              -70.584
    5      377              -70.584
    6       62              -70.584
    7      483              -70.584
    8     1712              -70.584
    9       13              -70.584
   10     1500              -70.584
```

11	1965	-70.584
12	1928	-70.584
13	648	-70.584
14	1280	-70.584
15	969	-70.584
16	991	-70.584
17	771	-70.584
18	1593	-70.584
19	1376	-70.584
20	456	-70.584

---- Cluster analysis ----

Lowest energy clusters (20 maximum):

Cluster	Frame	Cluster size	Energy (kcal/mol/asym. cell)
1	165	147	-70.584
2	1007	2	-70.581
3	1247	1	-70.549
4	1278	1	-70.401
5	1964	1	-70.160
6	1788	42	-69.967
7	895	14	-69.960
8	1144	1	-69.956
9	1728	1	-69.842
10	1977	1	-69.719
11	1175	28	-69.564
12	1899	1	-69.553
13	670	34	-69.141
14	1590	2	-69.140
15	1375	18	-69.025
16	1146	17	-68.817
17	1463	2	-68.803
18	1496	1	-68.780
19	1968	1	-68.742
20	448	2	-68.479

Calculation summary:

Number of frames searched : 2018
Number of clusters found : 426
Number of frames put into a cluster : 2018 (100 %).

##
Processing space group : C2/C
##

---- Packing ----

Space group : C 1 2/C 1
Random number seed : 240380207
Cooling factor : 0.00100
Number of trials made : 7000
Number of trials saved : 3578 (51.1%)
Maximum temperature achieved : 21767.2 K
Final temperature : 660.8 K

---- Cluster analysis ----

Lowest energy clusters (20 maximum):

Cluster	Frame	Cluster size	Energy (kcal/mol/asym. cell)
1	94	1	7.237
2	240	1	7.556
3	9	1	8.300
4	5	1	8.640
5	6	1	8.660
6	374	1	8.681
7	46	1	8.742
8	292	1	8.867
9	406	1	8.948
10	49	1	9.157
11	210	1	9.252
12	174	1	9.349
13	215	1	9.482
14	232	1	9.518
15	179	1	9.592
16	111	1	9.623
17	137	1	9.714
18	217	1	9.793
19	11	1	9.807
20	199	1	9.938

Calculation summary:

Number of frames searched : 3578
Number of clusters found : 587
Number of frames put into a cluster : 3578 (100 %).

---- Geometry optimization ----

Total number of frames : 587
Frames with lowest energy:

Order	Frame	Energy (kcal/mol/asym. cell)
1	200	-69.915
2	287	-69.095
3	148	-68.900
4	367	-68.859
5	227	-68.825
6	387	-68.763
7	454	-68.468
8	19	-68.468
9	175	-68.315
10	352	-68.166
11	1	-68.094
12	28	-68.071
13	476	-67.988
14	486	-67.625
15	51	-67.585
16	396	-67.582
17	16	-67.552
18	72	-67.552

19	554	-67.337
20	302	-67.337

---- Cluster analysis ----

Lowest energy clusters (20 maximum):

Cluster	Frame	Cluster size	Energy (kcal/mol/asym. cell)
1	200	1	-69.915
2	287	1	-69.095
3	148	1	-68.900
4	367	1	-68.859
5	227	1	-68.825
6	387	1	-68.763
7	454	2	-68.468
8	175	1	-68.315
9	352	1	-68.166
10	1	1	-68.094
11	28	1	-68.071
12	476	1	-67.988
13	486	1	-67.625
14	51	1	-67.585
15	396	1	-67.582
16	16	2	-67.552
17	554	2	-67.337
18	330	4	-67.240
19	354	1	-67.139
20	566	1	-67.109

Calculation summary:

Number of frames searched : 587
Number of clusters found : 470
Number of frames put into a cluster : 587 (100 %).

Task terminated : Wed Sep 04 17:27:41 2013
Total CPU time used : 7:49:17 hours

Termination status : Normal