Electronic Supplementary Material (ESI) for CrystEngComm.

Time for quartet: the stable 3:1 cocrystal formulation of FTDO and BTF – a high-energy-density material

Victor P. Zelenov, Nikita M. Baraboshkin, Dmitry V. Khakimov, Nikita V. Muravyev, Dmitry B. Meerov, Ivan A. Troyan, Tatyana S. Pivina, Alexandr V. Dzyabchenko, and Ivan V. Fedyanin

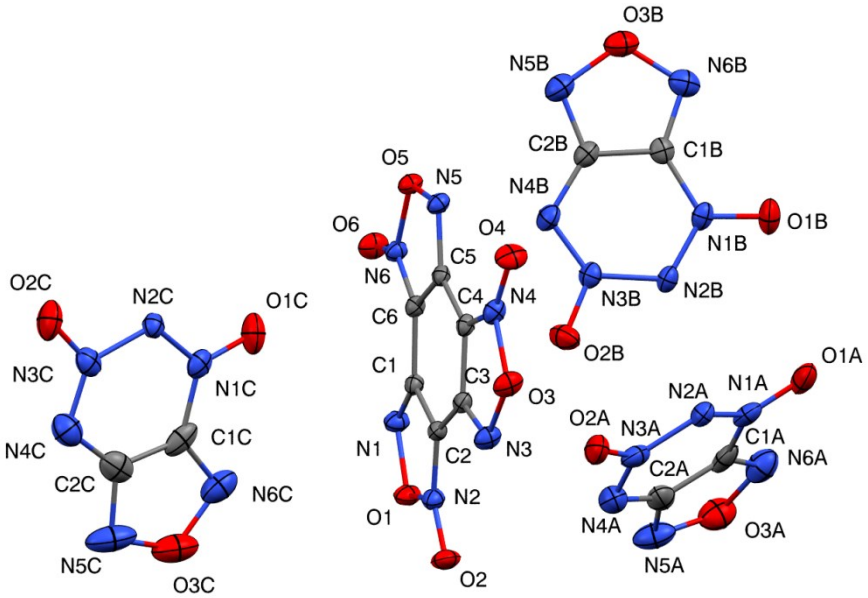

Figure S1. A representative part of unit cell of FTDO–BTF (3:1) cocrystal. Atoms are represented by thermal displacement ellipsoids from experimental X-Ray diffraction data.

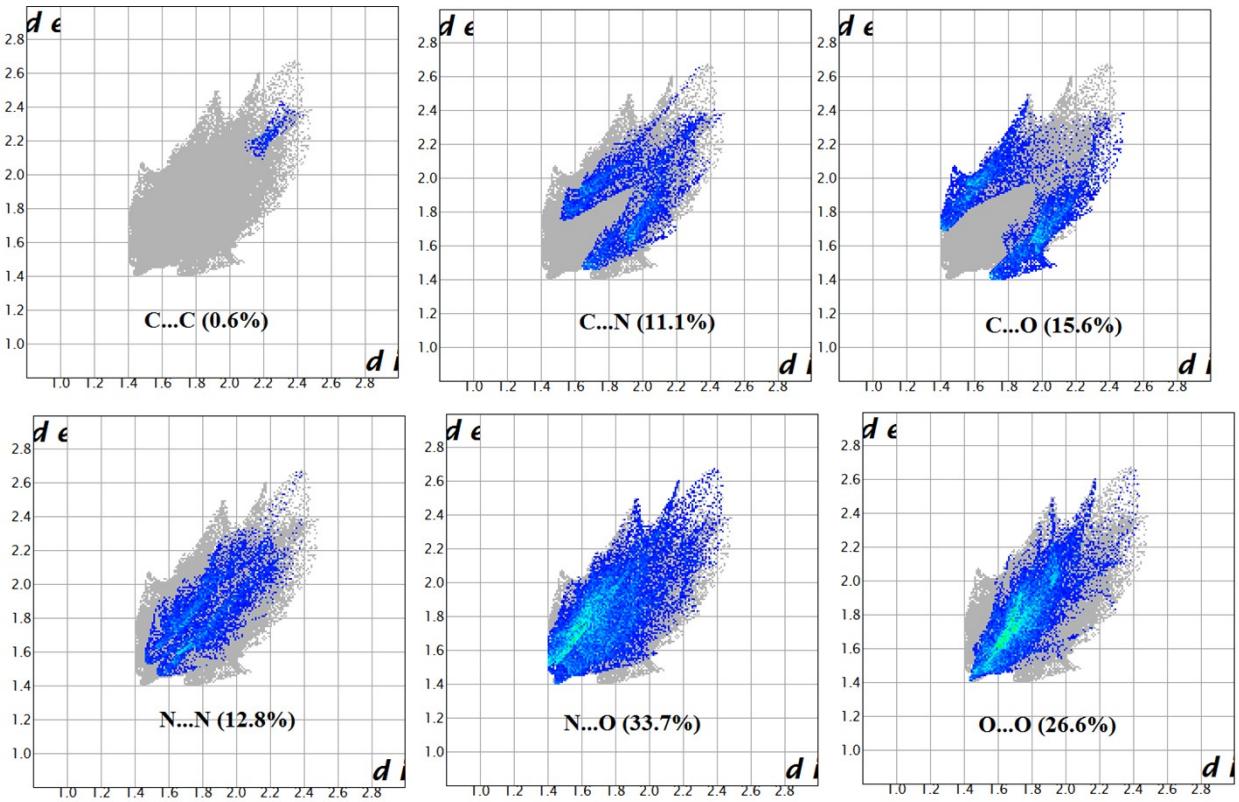

Figure S2. FTDO–BTF (1:1) calculated structure 2D-fingerprint plots.

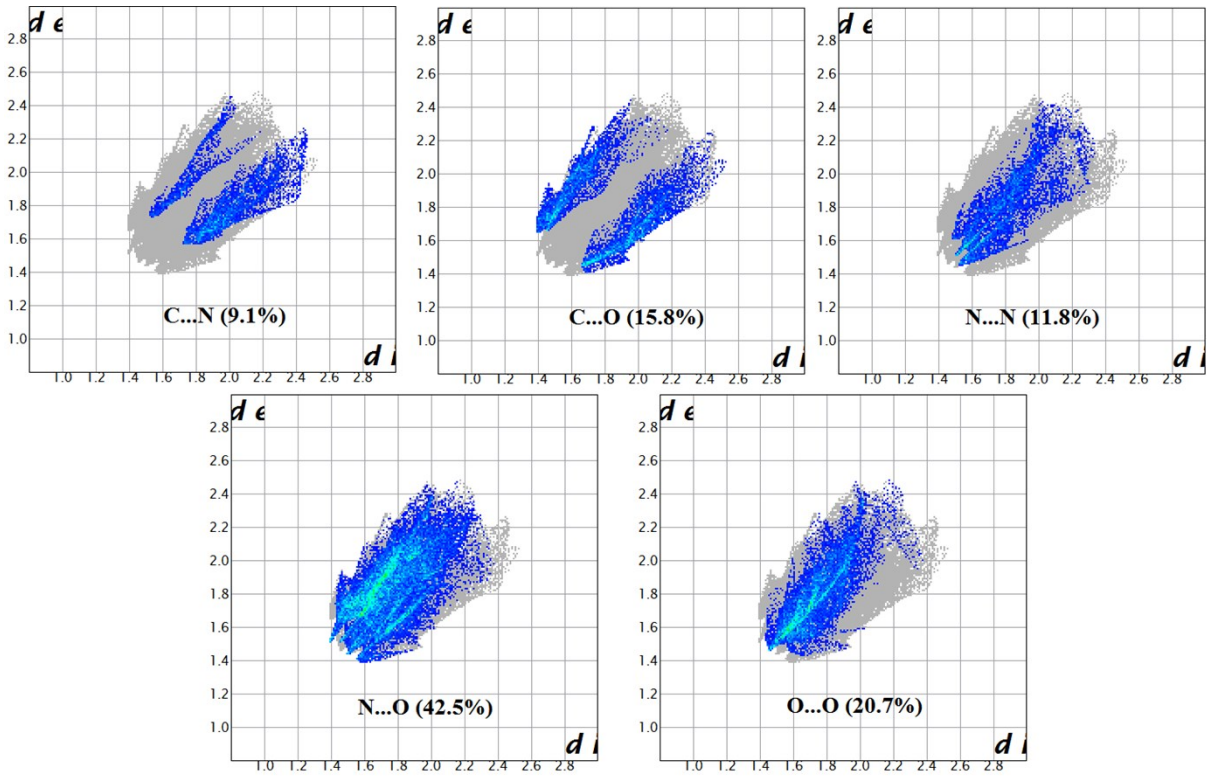

Figure S3. FTDO–BTF (2:1) calculated structure 2D-fingerprint plots.

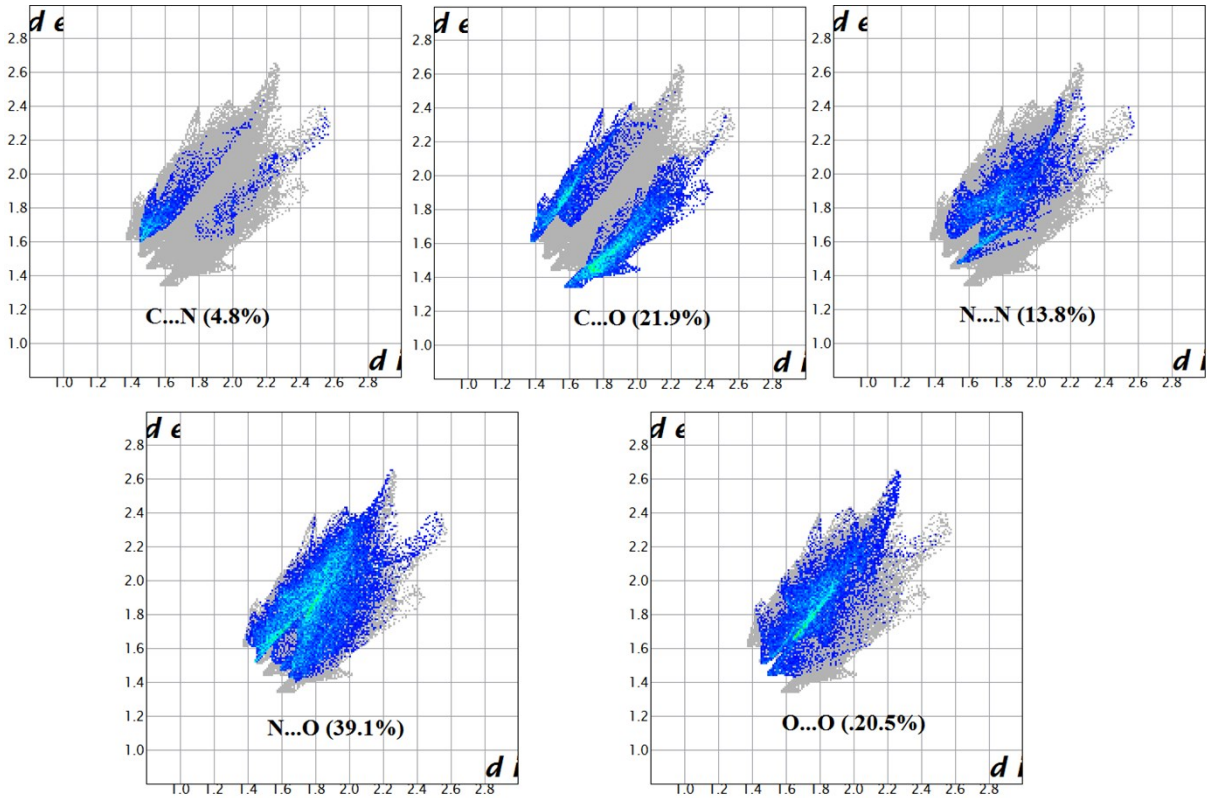

Figure S4. FTDO–BTF (3:1) calculated structure 2D-fingerprint plots.

Table S1. List of short contacts in the FTDO–BTF (3:1) cocrystal at 298 K.

Number	Atom1	Atom2	Length
1	O2B	O2B	2.907
2	O2A	N3B	2.911
3	N3A	O2D	2.912
4	C3	O2B	2.921
5	O2B	N3B	2.923
6	O5	O1A	2.941
7	O4	N2D	2.960
8	C2	O2B	2.963
9	N6D	O1A	2.970
10	O6	O2A	2.975
11	O4	C1A	2.988
12	O6	O1D	3.011
13	N6	N4A	3.012
14	O6	N2A	3.033
15	O4	N6A	3.038
16	C4	O2D	3.039
17	N2A	N1B	3.052
18	N3	C1B	3.063
19	O2	N6D	3.063
20	C5	O2D	3.081
21	N2A	N2D	3.087
22	N5	C1D	3.088
23	O6	C2B	3.113
24	C4	O1B	3.116
25	N1	C2A	3.123
26	N1	C1A	3.150
27	C3	O1B	3.152
28	O2	C1D	3.158
29	C6	O2A	3.169
30	C6	O1D	3.169
31	C1	O2A	3.170
32	O6	C1B	3.181
33	C1	O1D	3.190
34	O4	C2A	3.194
35	N5	C2D	3.221

Table S2. A comparison of the experimental vibrational spectra of BTF, FTDO and (3:1) cocrystal

FTDO		BTF		Cocrystal (3:1)		Frequency assignment[a]
Raman	**IR**	**Raman**	**IR**	**Raman**	**IR**	
115w				115w		
146w		145m		146vw		
		166w		170vw		
		186m				
		191s		194w		
214w		211w		219w		
233w				234w		
		290s		293s		
		314m				
328s				327s		
376w				377w		
		381s		385w		
407m				407m	408s	
410w				410m		
			415m			
422w						
		431w		430m		
			437s		443s	
		460s				
477s	477s			478s	477s	
		523s		525m		
552s	551s			552s	551s	
				554s		
		564w		566w		
		572vw	571w		573m	
589s	587s			589s	588s	
	600m			600w	599m	
632w	630m				631m	
			648s		653s	
679w	677s	679w		680w	677s	TDO-ring
724s	724s			726s	723s	
		732w	736m		738m	
	746m				746w	
		782s		785w		
		807w	806s	812vw	810s	
859m	853s			859m	853s	
	872s			871s	870s	
875s				874s		
					914m	
		936s	930w			
940s	940s			941s	940s	
		961w	961s		962s	
			997w			
1019s	1019s			1019s	1017s	
		1042w				

		1081m	1078s		1082s	
			1109w		1109w	
1149vs	1149s			1147s	1148s	TDO-ring
				1151vs		
				1175w	1178m	
1212m				1212s	1210m	
		1283s				
		1292m	1290s	1290w	1295s	
		1298m				
			1305m		1305s	
	1318s				1320s	
					1354m	
1409s				1412m	1410s	
	1421s	1419m	1417s	1422m	1419s	ν^{as} (N=N) FTDO
		1450m		1446w		
1457m				1455s		
	1460vs			1462w	1460s	
				1478vw		
1509w	1514vs			1510m	1508vs	
				1535m	1536s	
				1540s		
1544s	1543vs			1547s		ν^{s} (N=N) FTDO
		1564vs		1562w		
		1568s	1568vs	1570s		
		1577s			1578s	
1591s	1589s			1587s		
			1605s			
					1617w	
		1649s	1649vs	1657w	1656vs	
		1666w		1667w	1665vs	

[a] Frequency assignment is given for the key frequencies for FTDO accordingly literature data[1].

Table S3. The vibrational spectra of BTF

Raman			**IR**			
This work		Lit. [2]	This work		Lit.	
Exp.	Calc.		Exp.	Calc.	Bailey [3]	Katritzky [2]
	83w					
145m				102s		
166w						
186m		185m		186m		
191s	187s	190m				
211w						
290s	259s	290m				
314m	317s	320vw				
381s	382vs	380w		384s		
	410s		415m			420br
431w	421s	430w				
			437s	420s		440br

460s		465m				
523s	526vs	520w				
564w		564vw		556m		
572vw	601s	570w	571w	606m		570w
	648s		648s	648s		651s
679w						
732w	734s		736m		735	736w
782s	792m	780w				
807w	821s	810w	806s	819vs	807	810ms
936s	958s	935w	930w		935	935w
961w			961s		962	965s
	1004s		997w	1005vs		
1042w						
1081m	1084vs	1085w	1078s	1119s	1075	1082m
	1120s		1109w		1105	1105w
1283s	1303vs	1285w				
1292m			1290s		1287	1287w
1298m	1321vs					
			1305m	1320s	1304	1304w
1419m	1444vs	1420w	1417s	1444s	1416	1415m
1450m	1487vs	1455w				
					1508[a]	
					1540[a]	
1564vs						
1568s	1595vs	1570s	1568vs	1612vs	1572	1570s
1577s						
			1605s		1608	1608w
1649s	1721s	1650m	1649vs	1720vvs	1656	1656s
1666w	1746s					

[a] Possibly, the frequencies of an admixture.

Table S4. The vibrational spectra of FTDO

Raman		**IR**		Lit. [1]
This work		This work		
Exp.	Calc.	Exp.	Calc.	
				74[a]
115w[a]	102w		102w	
146w	162w		163w	146
214w[a]	208vw		209s	
				226[a]
233w[a]				234
328s	333m		333s	329
376w	356vw		357s	375
407m	396vw		396s	
410w[a]				
422w				418
477s	474s	477s	474s	479
552s	551s	551s	551s	548
589s	583vs	587s	583s	585
		600m[a]		

632w	616w	630m	617s	
679w	674w	677s	674s	676
	711w			
724s	738s	724s	738s	722
		746m[a]		
				843
859m	861s	853s	861s	855
875s	875s	872s	875s	871
	913s		913s	
940s	935s	940s	935vs	941
1019s	1037s	1019s	1037s	1016
1149vs	1159vs	1149s	1159s	1148
				1178[a]
1212m	1235s		1235s	1208
		1318s	1340s	1316
1409s[a]	1341m			
		1421s	1449vs	1420
1457m	1449s	1460vs	1496s	1460
1509w	1496vs	1514vs		1517
				1537[a]
1544s	1533s	1543vs	1533vvs	1548
1591s	1593s	1589s	1593vvs	1589
	1635vs		1635s	

[a] Apparently, the observed differences in the known and obtained FTDO spectra are due to crystal polymorphism.

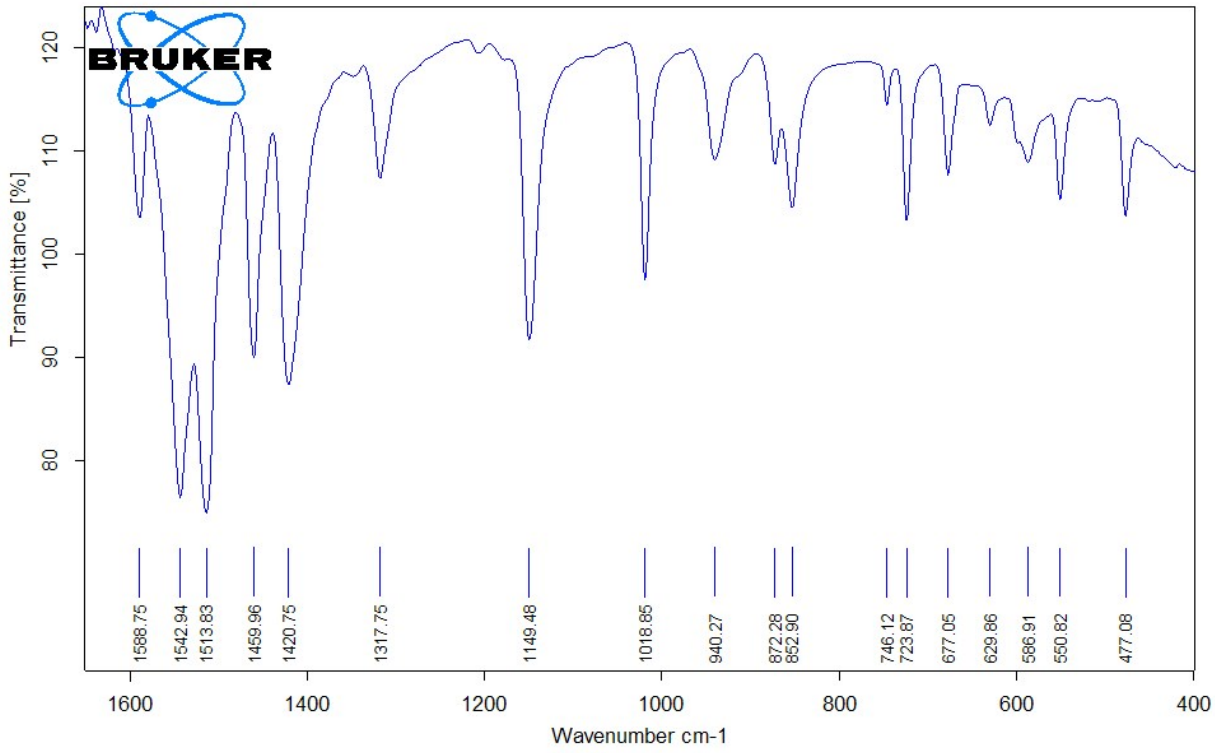

Figure S5. FTIR spectrum of FTDO (KBr).

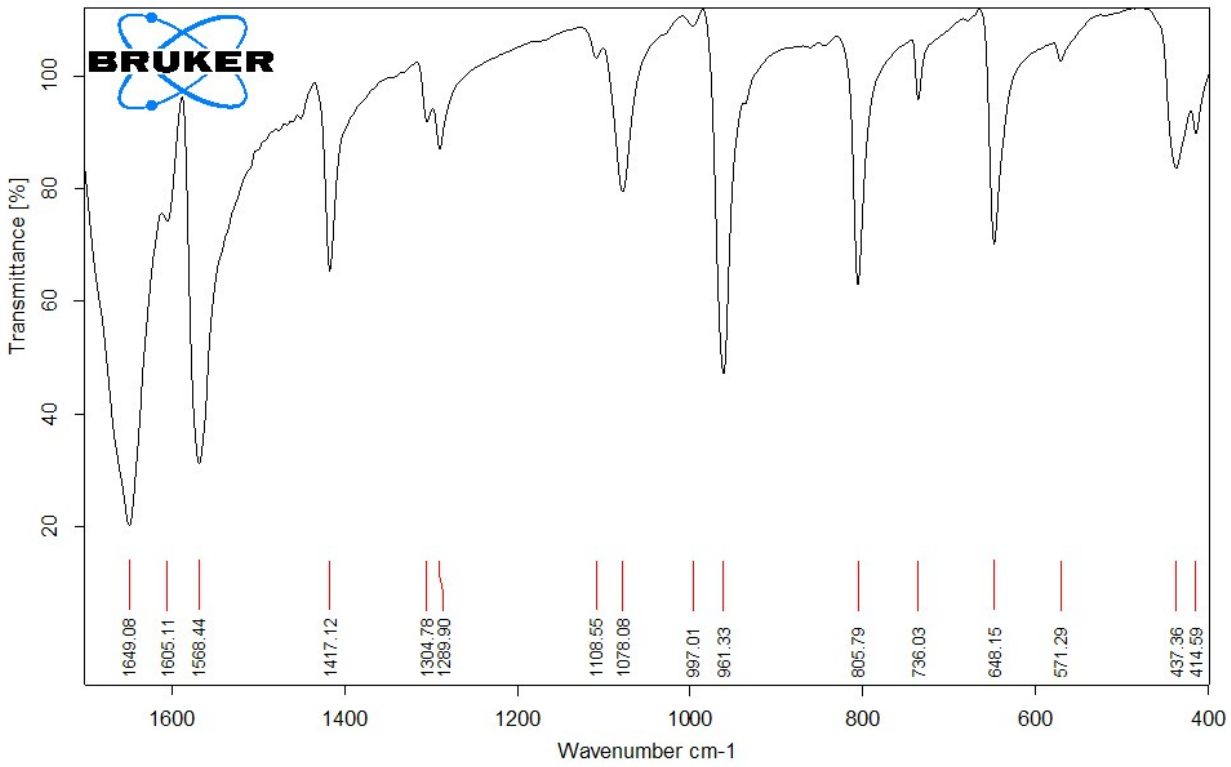

Figure S6. FTIR spectrum of BTF (KBr).

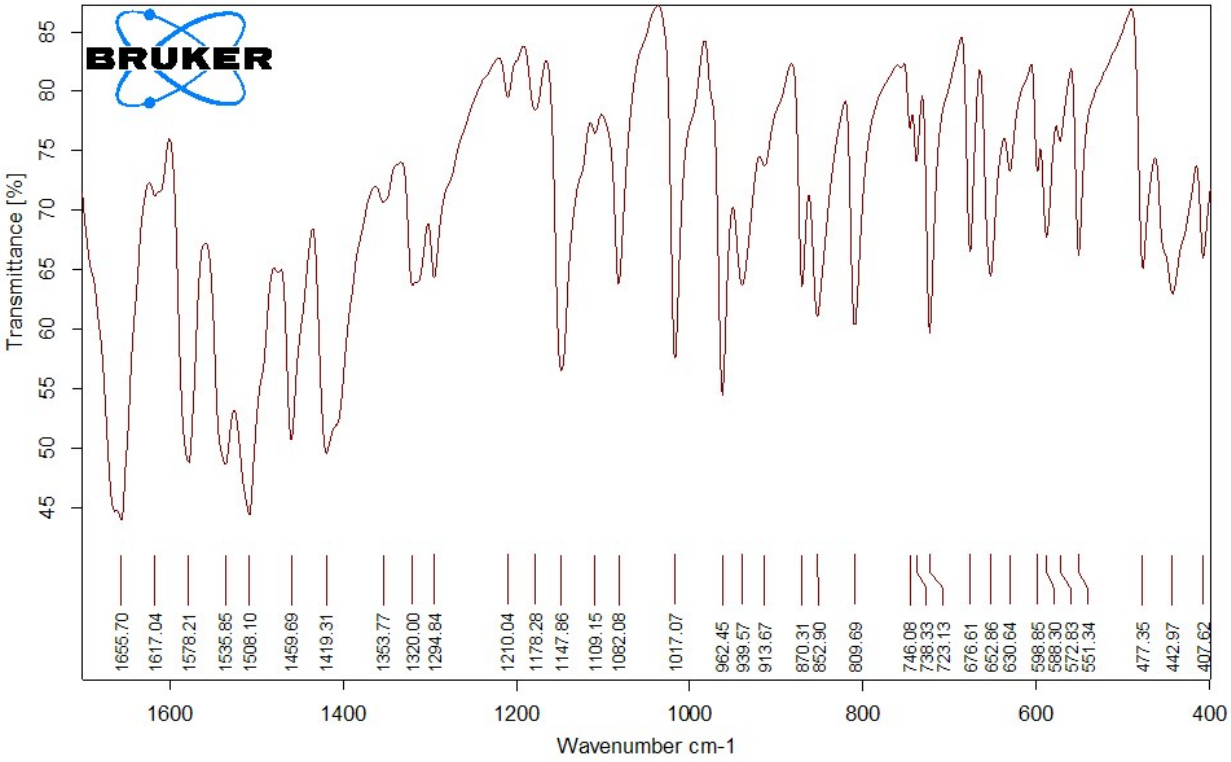

Figure S7. FTIR spectrum of FTDO–BTF (3:1) cocrystal (KBr).

[1] K. I. Rezchikova, A. M. Churakov, V. A. Shlyapochnikov, V. A. Tartakovsky, *Russ. Chem.*

Bull. Int. Ed., 1995, **44**, 2093–2095.
[2] N. Bacon, A. J. Boulton, A. R. Katritzky, *Trans. Faraday Soc.*, 1967, **63**, 833–835.
[3] A. S. Bailey, J. R. Case, *Tetrahedron*, 1958, **3** (2), 113–131.