Quest: structure and properties of BTF-nitrobenzenes cocrystals with different ratio of components

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In the supporting materials, models of the predicted cocrystal structures in .cif format and the coordinates of the atoms of the BTF-benzene solvate are presented.

Simulated and experimental structure of BTF-benzene solvate

Experimental

```
data_BTF-benzene(1:1)

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
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The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
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 'x, -y-1/2, z-1/2'

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_reflns_special_details
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 Reflections were merged by SHELXL according to the crystal
 class for the calculation of statistics and refinement.

 _reflns_Friedel_fraction is defined as the number of unique
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 _atom_site_occupancy
 _atom_site_site_symmetry_order
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C1F C 0.1351(6) -0.0573(9) 0.4143(6) 0.0442(18) Uani 1 1 d . . . . .
H1F H 0.061394 -0.098129 0.381293 0.053 Uiso 1 1 calc R U . . .
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C2F C 0.1892(7) 0.0038(9) 0.3604(6) 0.048(2) Uani 1 1 d . . . . .
H2F H 0.152876 0.006106 0.289683 0.058 Uiso 1 1 calc R U . . .
C3F C 0.2978(6) 0.0619(9) 0.4115(6) 0.0449(18) Uani 1 1 d . . . . .
H3F H 0.335147 0.103845 0.375028 0.054 Uiso 1 1 calc R U . . .
C4F C 0.3505(6) 0.0590(8) 0.5128(6) 0.0425(18) Uani 1 1 d . . . . .
H4F H 0.424438 0.098145 0.546117 0.051 Uiso 1 1 calc R U . . .
C5F C 0.2981(6) 0.0001(8) 0.5678(6) 0.0407(17) Uani 1 1 d . . . . .
H5F H 0.334893 -0.000742 0.638543 0.049 Uiso 1 1 calc R U . . .
C6F C 0.1915(6) -0.0573(9) 0.5178(6) 0.0420(17) Uani 1 1 d . . . . .
H6F H 0.155004 -0.098362 0.555206 0.050 Uiso 1 1 calc R U . . .
C1A C 0.1765(5) 0.4759(11) 0.3984(4) 0.0342(12) Uani 0.5 1 d DG . P A 1
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O1A O 0.1686(8) 0.5519(15) 0.2411(8) 0.0760(18) Uani 0.5 1 d D . P A 1
O2A O 0.5222(9) 0.6679(17) 0.6543(7) 0.0760(18) Uani 0.5 1 d D . P A 1
O3A O 0.0936(8) 0.3113(16) 0.5949(7) 0.0760(18) Uani 0.5 1 d D . P A 1
O4A O 0.3726(13) 0.676(3) 0.3435(14) 0.0760(18) Uani 0.25 1 d D . P A 1
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C1B C 0.2149(6) 0.5180(12) 0.3838(4) 0.0342(12) Uani 0.5 1 d DG . P B 2
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C4B C 0.2923(6) 0.4817(12) 0.5887(4) 0.0342(12) Uani 0.5 1 d DG . P B 2
C5B C 0.1864(6) 0.4274(12) 0.5249(6) 0.0342(12) Uani 0.5 1 d DG . P B 2
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N1B N 0.2138(10) 0.5592(19) 0.2940(6) 0.0757(17) Uani 0.5 1 d D . P B 2
N2B N 0.3849(8) 0.6458(18) 0.4075(7) 0.0757(17) Uani 0.5 1 d D . P B 2
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N5B N 0.1005(7) 0.3489(19) 0.5350(9) 0.0757(17) Uani 0.5 1 d D . P B 2
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O1B O 0.3164(8) 0.6487(17) 0.2920(7) 0.0760(18) Uani 0.5 1 d D . P B 2
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O3B O 0.0023(9) 0.3165(16) 0.4308(7) 0.0760(18) Uani 0.5 1 d D . P B 2
O4B O 0.5236(10) 0.6682(17) 0.6114(10) 0.0760(18) Uani 0.5 1 d D . P B 2

Simulated

data_ BTF-benzene(1:1)_-4.112587E+01

```
_chemical_name_systematic
;RAS BTFO_C3H

E(total)=-1.88437E+01 E(coul)=-1.00109E+01 E(vdW)=-8.83278E+00 Density= 1.60557
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_cell_length_c   14.799
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_cell_formula_units_Z  4
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_symmetry_Int_Tables_number  14
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_atom_site_fract_x
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_atom_site_fract_z
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C2A       0.15338   0.01086  -0.09896                    #  2
C3A       0.12586   0.08305  -0.02556                    #  3
C4A       0.20075   0.08604   0.07368                    #  4
C5A       0.30318   0.01682   0.09952                    #  5
C6A       0.33070  -0.05537   0.02612                    #  6
H7A       0.27722  -0.11450  -0.13020                    #  7
H8A       0.09514   0.00854  -0.17613                    #  8
H9A       0.04620   0.13688  -0.04565                    #  9
H10A      0.17934   0.14218   0.13076                    # 10
H11A      0.36142   0.01914   0.17669                    # 11
H12A      0.41036  -0.10920   0.04621                    # 12
C1        0.23252  -0.06820   0.61117                   # 49
C2        0.16610  -0.05880   0.50658                   # 50
C3        0.20577   0.00481   0.43635                   # 51
C4        0.31521   0.05957   0.47399                   # 52
C5        0.38512   0.05254   0.57857                   # 53
C6        0.34211  -0.01163   0.64552                   # 54
N7        0.06956  -0.11699   0.49231                    # 55
O8        0.07897  -0.16339   0.59353                    # 56
N'9       0.18053  -0.12972   0.66133                    # 57
N'10      0.15684   0.02212   0.33939                    # 58
```

```
O11       0.23026   0.08803   0.30874                    # 59
N12       0.33385   0.11251   0.39681                    # 60
N'13      0.48604   0.09673   0.62537                    # 61
O14       0.51418   0.06450   0.72382                    # 62
N15       0.42000  -0.00638   0.73697                    # 63
O16       0.40966   0.17039   0.38465                    # 64
O17      -0.01542  -0.13781   0.42148                    # 65
O18       0.42917  -0.04344   0.81996                    # 66
#END
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Simulated cocrystal structures of BTF-Nitrobenzene

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_chemical_name_systematic
;RAS

E(total)=-4.22904E+01 E(coul)=-1.13322E+01 E(vdW)=-3.13261E+01 Density= 1.71976
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C2a       0.03448  -0.20968   0.31914                    #  2
C3a       0.23290  -0.17050   0.30887                    #  3
C4a       0.23727  -0.11960   0.39300                    #  4
C5a       0.05184  -0.10692   0.48572                    #  5
```

```
C6a      -0.14129  -0.14725   0.49202                          #  6
N7a      -0.01330  -0.25933   0.25381                          #  7
O8a      -0.24360  -0.27937   0.30862                          #  8
N9a      -0.31614  -0.24019   0.40259                          #  9
N10a      0.41861  -0.17344   0.23246                          # 10
O11a      0.55300  -0.12538   0.26180                          # 11
N12a      0.43390  -0.09002   0.36724                          # 12
N13a      0.02799  -0.06290   0.56912                          # 13
O14a     -0.17894  -0.07178   0.63376                          # 14
N15a     -0.29014  -0.12719   0.58312                          # 15
O16a      0.52572  -0.04529   0.40733                          # 16
O17a      0.08118  -0.28834   0.16854                          # 17
O18a     -0.47645  -0.14290   0.62830                          # 18
C1       -0.29420   0.11282   0.11002                         # 37
C2       -0.16733   0.15356   0.02318                         # 38
C3        0.05553   0.14048  -0.01687                         # 39
C11       0.15294   0.08665   0.02954                          # 40
C12       0.02323   0.04671   0.11605                          # 41
C6       -0.19928   0.05879   0.15734                         # 42
H7       -0.46722   0.12308   0.14099                         # 43
H8        0.15370   0.17219  -0.08431                         # 44
H12      -0.29288   0.02627   0.22468                          # 45
H13       0.32506   0.07515   0.00046                          # 46
H14      -0.24228   0.19559  -0.01334                          # 47
N9        0.12499  -0.01055   0.16586                         # 60
O10       0.00380  -0.05184   0.23037                          # 61
O11       0.32483  -0.01358   0.14001                          # 62
#END

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_chemical_name_systematic
;RAS b3lyp-d3

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C2a       0.32757   0.01668   0.15934                    #  2
C3a       0.26771  -0.08764   0.16563                    #  3
C4a       0.21008  -0.08398   0.26019                    #  4
C5a       0.21052   0.01938   0.34734                    #  5
C6a       0.27126   0.12066   0.33708                    #  6
N7a       0.38726   0.03702   0.08193                    #  7
O8a       0.42811   0.16113   0.12264                    #  8
N9a       0.38976   0.20564   0.22131                    #  9
N10a      0.25628  -0.18999   0.09676                    # 10
O11a      0.19151  -0.25809   0.14164                    # 11
N12a      0.16115  -0.18846   0.24898                    # 12
N13a      0.16286   0.03772   0.43854                    # 13
O14a      0.18929   0.15032   0.49233                    # 14
N15a      0.26049   0.20480   0.42569                    # 15
O16a      0.10351  -0.23358   0.30208                    # 16
O17a      0.41242  -0.01833  -0.00503                    # 17
O18a      0.29298   0.30527   0.45955                    # 18
C1        0.00093   0.30419  -0.07160                   # 37
C2        0.02548   0.31474  -0.18181                   # 38
C3        0.08290   0.22153  -0.23700                   # 39
C11       0.11611   0.11729  -0.18246                    # 40
C12       0.09072   0.10876  -0.07257                    # 41
C6        0.03356   0.20054  -0.01588                   # 42
H7       -0.04366   0.37669  -0.02892                    # 43
H8        0.10187   0.22994  -0.32259                   # 44
H12       0.01586   0.18950   0.06947                    # 45
H13       0.16069   0.04345  -0.22278                    # 46
H14      -0.00017   0.39576  -0.22478                    # 47
N9        0.12556  -0.00127  -0.01421                   # 59
O10       0.10225  -0.00682   0.08277                    # 60
O11       0.17592  -0.08112  -0.06590                    # 61
C1        0.52284   0.26294   0.32473                   # 65
C2        0.55910   0.29111   0.21896                   # 66
C3        0.62564   0.22045   0.17455                   # 67
C11       0.65634   0.12129   0.23548                    # 68
C12       0.61921   0.09493   0.34077                    # 69
C6        0.55281   0.16409   0.38673                   # 70
H7        0.47118   0.31795   0.35903                   # 71
```

```
H8       0.65369   0.24250   0.09240                          # 72
H12       0.52614   0.13982   0.46888                          # 73
H13       0.70777   0.06473   0.20353                          # 74
H14       0.53546   0.36827   0.17105                          # 75
N9       0.65132  -0.00987   0.40583                          # 87
O10       0.61758  -0.03143   0.49857                          # 88
O11       0.70997  -0.06963   0.36359                          # 89
#END



data_ BTF-nitrobenzene(1:3)_-7.57108E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-7.57108E+01 E(coul)=-1.70983E+01 E(vdW)=-5.86124E+01 Density= 1.53113
;
_cell_length_a   10.546
_cell_length_b   11.215
_cell_length_c   13.065
_cell_angle_alpha   109.28
_cell_angle_beta    95.02
_cell_angle_gamma   108.77
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1a      -0.53070  -0.58578  -0.37497                          #  1
C2a      -0.65602  -0.64774  -0.34584                          #  2
C3a      -0.67824  -0.59847  -0.23494                          #  3
C4a      -0.56978  -0.48356  -0.15264                          #  4
C5a      -0.44166  -0.41745  -0.17758                          #  5
C6a      -0.42481  -0.47040  -0.28902                          #  6
N7a      -0.73825  -0.75111  -0.43674                          #  7
O8a      -0.65707  -0.75042  -0.52484                          #  8
N9a      -0.53243  -0.64671  -0.47998                          #  9
N10a     -0.78530  -0.64249  -0.19439                          # 10
O11a     -0.75347  -0.56014  -0.08493                          # 11
```

N12a	-0.61191	-0.45575	-0.05750	# 12
N13a	-0.33287	-0.31250	-0.11313	# 13
O14a	-0.24006	-0.29113	-0.17773	# 14
N15a	-0.30044	-0.39484	-0.29326	# 15
O16a	-0.56428	-0.37244	0.03627	# 16
O17a	-0.85263	-0.83610	-0.46002	# 17
O18a	-0.23369	-0.39316	-0.36375	# 18
C1	-0.95245	-1.11455	-0.27585	# 37
C2	-0.86504	-0.97916	-0.24619	# 38
C3	-0.73462	-0.92948	-0.17848	# 39
C11	-0.69074	-1.01467	-0.13999	# 40
C12	-0.77964	-1.14928	-0.17063	# 41
C6	-0.91012	-1.20106	-0.23806	# 42
H7	-1.05368	-1.15289	-0.32844	# 43
H8	-0.66693	-0.82431	-0.15556	# 44
H12	-0.97528	-1.30641	-0.25948	# 45
H13	-0.59039	-0.97941	-0.08743	# 46
H14	-0.89863	-0.91225	-0.27591	# 47
N9	-0.73401	-1.24016	-0.13026	# 59
O10	-0.81421	-1.35860	-0.15836	# 60
O11	-0.61841	-1.19225	-0.07084	# 61
C1	-0.95288	-1.20825	-0.93788	# 65
C2	-0.86526	-1.07588	-0.91890	# 66
C3	-0.73029	-1.02457	-0.85874	# 67
C11	-0.68206	-1.10514	-0.81720	# 68
C12	-0.77127	-1.23682	-0.83716	# 69
C6	-0.90625	-1.29013	-0.89692	# 70
H7	-1.05765	-1.24786	-0.98462	# 71
H8	-0.66244	-0.92175	-0.84410	# 72
H12	-0.97144	-1.39307	-0.91014	# 73
H13	-0.57814	-1.06852	-0.77030	# 74
H14	-0.90222	-1.01257	-0.95105	# 75
N9	-0.72106	-1.32280	-0.79349	# 87
O10	-0.80162	-1.43871	-0.81212	# 88
O11	-0.60154	-1.27361	-0.74098	# 89
C1	-0.90187	-1.26833	-0.59457	# 93
C2	-0.81348	-1.13559	-0.57363	# 94
C3	-0.69045	-1.07549	-0.49425	# 95
C11	-0.65498	-1.14758	-0.43535	# 96
C12	-0.74470	-1.27980	-0.45762	# 97
C6	-0.86792	-1.34180	-0.53638	# 98
H7	-0.99735	-1.31478	-0.65625	# 99
H8	-0.62198	-0.97240	-0.47814	#100
H12	-0.93406	-1.44477	-0.55059	#101
H13	-0.56050	-1.10404	-0.37334	#102
H14	-0.84053	-1.07887	-0.61925	#103
N9	-0.70797	-1.35684	-0.39566	#115

```
O10      -0.78873  -1.47340  -0.41670                        #116
O11      -0.59869  -1.30007  -0.32653                        #117
#END



data_ BTF-nitrobenzene(2:1)_-6.88951E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-6.88951E+01 E(coul)=-1.40536E+01 E(vdW)=-5.48415E+01 Density= 1.76762
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_cell_length_a    6.488
_cell_length_b   11.024
_cell_length_c   16.924
_cell_angle_alpha   100.74
_cell_angle_beta    95.08
_cell_angle_gamma    94.68
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1a       0.56257   0.14336  -0.35200                       #  1
C2a       0.67587   0.25612  -0.30821                       #  2
C3a       0.60055   0.33076  -0.23963                       #  3
C4a       0.40547   0.28874  -0.21569                       #  4
C5a       0.28528   0.17597  -0.25766                       #  5
C6a       0.36706   0.10523  -0.32540                       #  6
N7a       0.84949   0.27324  -0.34277                       #  7
O8a       0.83857   0.16441  -0.41096                       #  8
N9a       0.65926   0.09043  -0.41203                       #  9
N10a      0.68321   0.43519  -0.19322                       # 10
O11a      0.54898   0.46696  -0.13711                       # 11
N12a      0.36655   0.37077  -0.15187                       # 12
N13a      0.10593   0.12448  -0.24405                       # 13
O14a      0.06085   0.01873  -0.30123                       # 14
N15a      0.23236   0.00608  -0.35466                       # 15
O16a      0.22887   0.38211  -0.10820                       # 16
O17a      0.99791   0.35038  -0.33149                       # 17
```

```
O18a      0.22162  -0.08239  -0.40961                    # 18
C1a      -0.10904  -0.62647   0.28002                    # 37
C2a       0.07217  -0.69077   0.26883                    # 38
C3a       0.18426  -0.73393   0.33377                    # 39
C4a       0.10876  -0.71057   0.41151                    # 40
C5a      -0.07283  -0.64629   0.42602                    # 41
C6a      -0.17852  -0.60535   0.35946                    # 42
N7a       0.10785  -0.69992   0.19184                    # 43
O8a      -0.06190  -0.63747   0.15526                    # 44
N9a      -0.18627  -0.59570   0.21314                    # 45
N10a      0.35091  -0.79357   0.33412                    # 46
O11a      0.39329  -0.81234   0.41094                    # 47
N12a      0.23424  -0.75783   0.46177                    # 48
N13a     -0.16225  -0.61743   0.49255                    # 49
O14a     -0.32899  -0.55689   0.47360                    # 50
N15a     -0.33969  -0.54895   0.38619                    # 51
O16a      0.24467  -0.76488   0.53240                    # 52
O17a      0.23551  -0.74363   0.15005                    # 53
O18a     -0.47778  -0.49819   0.35735                    # 54
C1       0.54781   0.23887   0.00276                    # 73
C2       0.74142   0.25100  -0.02672                    # 74
C3       0.79006   0.16371  -0.09175                    # 75
C4       0.64568   0.06386  -0.12770                    # 76
C5       0.45362   0.05366  -0.09729                    # 77
C6       0.40171   0.13956  -0.03252                    # 78
H7       0.51041   0.30677   0.05326                    # 79
H8       0.94050   0.17333  -0.11453                    # 80
N9       0.29989  -0.05176  -0.13499                    # 81
O10      0.13136  -0.05888  -0.10715                    # 82
O11      0.34910  -0.12644  -0.19210                    # 83
H12      0.25039   0.12745  -0.01116                    # 84
H13      0.67841  -0.00535  -0.17815                    # 85
H14      0.85462   0.32861   0.00104                    # 86
#END
```

```
data___ BTF-nitrobenzene(3:1)____-9.22013E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-9.22013E+01 E(coul)=-1.98483E+01 E(vdW)=-7.23530E+01 Density= 1.79180
;
_cell_length_a   10.067
_cell_length_b   24.066
_cell_length_c    6.730
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_cell_angle_alpha    90.00
_cell_angle_beta     91.24
_cell_angle_gamma    90.00
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P 21    '
_symmetry_Int_Tables_number   4
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1a       0.21699   0.03869  -0.28354                    #  1
C2a       0.09375   0.01847  -0.21021                    #  2
C3a       0.01140  -0.01993  -0.32126                    #  3
C4a       0.05652  -0.03783  -0.51090                    #  4
C5a       0.17974  -0.01876  -0.59156                    #  5
C6a       0.25784   0.01937  -0.47526                    #  6
N7a       0.07586   0.04142  -0.03298                    #  7
O8a       0.19531   0.07732   0.00075                    #  8
N9a       0.27562   0.07312  -0.15884                    #  9
N10a     -0.10285  -0.04236  -0.27698                    # 10
O11a     -0.13843  -0.07571  -0.43274                    # 11
N12a     -0.03376  -0.07273  -0.58639                    # 12
N13a      0.23535  -0.03075  -0.76055                    # 13
O14a      0.35125  -0.00161  -0.76438                    # 14
N15a      0.36602   0.03131  -0.57700                    # 15
O16a     -0.04692  -0.09957  -0.73730                    # 16
O17a     -0.00808   0.03939   0.09249                    # 17
O18a      0.46313   0.06018  -0.55156                    # 18
C1a       0.68383   0.16437   0.27484                    # 37
C2a       0.72516   0.10983   0.33375                    # 38
C3a       0.70435   0.06201   0.20833                    # 39
C4a       0.63996   0.07042   0.01918                    # 40
C5a       0.59641   0.12443  -0.04727                    # 41
C6a       0.61947   0.17056   0.08298                    # 42
N7a       0.78157   0.11374   0.51379                    # 43
O8a       0.77322   0.17406   0.56460                    # 44
N9a       0.71246   0.20166   0.41112                    # 45
N10a      0.73549   0.00977   0.23853                    # 46
O11a      0.69388  -0.01855   0.07339                    # 47
N12a      0.63114   0.02129  -0.07070                    # 48
N13a      0.53664   0.13940  -0.21375                    # 49
O14a      0.51748   0.19531  -0.20208                    # 50
```

N15a 0.57189 0.21579 -0.00719 # 51
O16a 0.58752 0.00419 -0.22782 # 52
O17a 0.83257 0.08196 0.63165 # 53
O18a 0.56450 0.26467 0.03207 # 54
C1a -0.18589 -0.21599 0.04656 # 73
C2a -0.28002 -0.19954 0.19148 # 74
C3a -0.30175 -0.23138 0.36897 # 75
C4a -0.22540 -0.28096 0.39791 # 76
C5a -0.12940 -0.29937 0.25671 # 77
C6a -0.11162 -0.26624 0.08285 # 78
N7a -0.33654 -0.15258 0.12861 # 79
O8a -0.27226 -0.14048 -0.06467 # 80
N9a -0.18216 -0.18111 -0.10278 # 81
N10a -0.38292 -0.22247 0.51527 # 82
O11a -0.36458 -0.26506 0.64625 # 83
N12a -0.26113 -0.30348 0.56917 # 84
N13a -0.05196 -0.34315 0.25976 # 85
O14a 0.01980 -0.34119 0.09066 # 86
N15a -0.01937 -0.29067 -0.02555 # 87
O16a -0.23035 -0.34420 0.66463 # 88
O17a -0.42008 -0.12117 0.18928 # 89
O18a 0.03339 -0.28137 -0.18166 # 90
C1 -0.41563 0.38228 0.37558 #109
C2 -0.36588 0.39563 0.18928 #110
C3 -0.23912 0.37803 0.13657 #111
C4 -0.16135 0.34701 0.26955 #112
C5 -0.21301 0.33420 0.45448 #113
C6 -0.33912 0.35130 0.51026 #114
H7 -0.51409 0.39600 0.41616 #115
H8 -0.20071 0.38844 -0.00818 #116
N9 -0.13135 0.30139 0.59614 #117
O10 -0.17899 0.29056 0.75853 #118
O11 -0.02034 0.28674 0.54370 #119
H12 -0.37468 0.34026 0.65569 #120
H13 -0.06280 0.33274 0.23339 #121
H14 -0.42601 0.41979 0.08497 #122
#END

Simulated cocrystal structures of BTF-1,2-dinitrobenzene

data____ BTF-1,2-dinitrobenzene(1:1)___-1.54400E+02
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-1.54400E+02 E(coul)=-1.64085E+02 E(vdW)=-3.07831E+01 Density= 1.79769
;

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_cell_length_a   15.552
_cell_length_b    6.992
_cell_length_c    9.586
_cell_angle_alpha    90.00
_cell_angle_beta     48.14
_cell_angle_gamma    90.00
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P 21    '
_symmetry_Int_Tables_number   4
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,1/2+y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       0.24421  -0.17803   0.18787                    #  1
C2       0.32748  -0.13979   0.20433                    #  2
C3       0.32737   0.03554   0.28322                    #  3
C4       0.24017   0.17386   0.34624                    #  4
C5       0.15436   0.14249   0.33289                    #  5
C6       0.15829  -0.03406   0.25342                    #  6
N7       0.39760  -0.29010   0.13607                    #  7
O8       0.35340  -0.42525   0.07566                    #  8
N'9      0.26019  -0.34555   0.11235                    #  9
N'10     0.39630   0.09317   0.30854                    # 10
O11      0.35871   0.26978   0.38833                    # 11
N12      0.25616   0.32278   0.41310                    # 12
N'13     0.06945   0.25238   0.38309                    # 13
O14      0.01383   0.15547   0.33999                    # 14
N15      0.07218  -0.03268   0.25481                    # 15
O16      0.20975   0.47540   0.48219                    # 16
O17      0.48062  -0.33472   0.11525                    # 17
O18      0.03556  -0.14068   0.20654                    # 18
C1a      0.37251   0.05567   0.75385                    # 37
C2a      0.31085  -0.05813   0.72793                    # 38
C3a      0.20882   0.00968   0.77836                    # 39
C4a      0.16952   0.19289   0.85120                    # 40
C5a      0.23182   0.30786   0.87589                    # 41
C6a      0.33269   0.23903   0.82835                    # 42
H10a     0.45129  -0.00071   0.71352                    # 43
H11a     0.38113   0.32799   0.84780                    # 44
H12a     0.09017   0.24162   0.88898                    # 45
H13a     0.20082   0.45051   0.93345                    # 46
N7a      0.36204  -0.24381   0.63200                    # 59
```

```
O8a       0.41745  -0.32873   0.66192                          # 60
O9a       0.34972  -0.29387   0.52371                          # 61
N14a      0.14396  -0.12502   0.76714                          # 66
O15a      0.13390  -0.28658   0.82613                          # 67
O16a      0.10115  -0.06621   0.70447                          # 68
#END


data_ BTF-1,2-dinitrobenzene(1:2)_-6.71698E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-6.71698E+01 E(coul)=-1.66468E+01 E(vdW)=-5.05229E+01 Density= 1.67703
;
_cell_length_a    8.000
_cell_length_b   11.995
_cell_length_c   13.926
_cell_angle_alpha   108.04
_cell_angle_beta    101.05
_cell_angle_gamma   105.87
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.62504   0.51376  -0.18748                         #  1
C2        0.80999   0.54979  -0.12589                         #  2
C3        0.92004   0.47511  -0.15346                         #  3
C4        0.83854   0.36148  -0.24592                         #  4
C5        0.65300   0.32093  -0.31066                         #  5
C6        0.54956   0.39853  -0.27979                         #  6
N7        0.85094   0.65780  -0.04541                         #  7
O8        0.68054   0.68754  -0.06010                         #  8
N'9       0.55055   0.59509  -0.14825                         #  9
N'10      1.08950   0.49389  -0.10654                         # 10
O11       1.12793   0.39513  -0.16474                         # 11
N12       0.96310   0.30816  -0.25629                         # 12
N'13      0.55804   0.22083  -0.39681                         # 13
O14       0.38962   0.22714  -0.42676                         # 14
N15       0.38404   0.34385  -0.34991                         # 15
```

```
O16       0.96943   0.21406  -0.31788                    # 16
O17       0.98331   0.72894   0.02898                    # 17
O18       0.24536   0.36681  -0.36270                    # 18
C1a      -0.04851  -0.08653  -0.37595                    # 37
C2a      -0.10456  -0.20388  -0.36989                    # 38
C3a      -0.00369  -0.28196  -0.39186                    # 39
C4a       0.15547  -0.24178  -0.41780                    # 40
C5a       0.21270  -0.12361  -0.42308                    # 41
C6a       0.11043  -0.04648  -0.40280                    # 42
H10a     -0.12947  -0.02806  -0.35852                     # 43
H11a      0.15444   0.04532  -0.40708                     # 44
H12a      0.23089  -0.30432  -0.43440                     # 45
H13a      0.33653  -0.09257  -0.44375                     # 46
N7a      -0.26304  -0.23657  -0.33110                    # 57
O8a      -0.39010  -0.20489  -0.36197                    # 58
O9a      -0.25209  -0.28775  -0.26761                    # 59
N14a      -0.06764  -0.41208  -0.39758                    # 63
O15a      -0.23122  -0.47261  -0.43838                    # 64
O16a      0.04933  -0.45114  -0.36521                    # 65
C1a      -0.44013   0.12509   0.14180                    # 69
C2a      -0.49742   0.00950   0.15092                    # 70
C3a      -0.39176  -0.06635   0.13780                    # 71
C4a      -0.22679  -0.02562   0.11771                    # 72
C5a      -0.16840   0.09082   0.10938                    # 73
C6a      -0.27528   0.16566   0.12079                    # 74
H10a      -0.52489   0.18185   0.15233                    # 75
H11a      -0.23036   0.25610   0.11411                    # 76
H12a      -0.14776  -0.08642   0.10793                    # 77
H13a      -0.04000   0.12228   0.09326                    # 78
N7a      -0.66319  -0.02341   0.18346                    # 89
O8a      -0.78929   0.00466   0.14509                    # 90
O9a      -0.65904  -0.07110   0.24963                    # 91
N14a      -0.45569  -0.19501   0.13547                    # 95
O15a      -0.61746  -0.25818   0.09003                    # 96
O16a      -0.34001  -0.23041   0.17521                    # 97
#END
```

```
data_ BTF-1,2-dinitrobenzene(1:3)_-8.68657E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-8.68657E+01 E(coul)=-2.39434E+01 E(vdW)=-6.29223E+01 Density= 1.63144
;
_cell_length_a   13.145
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_cell_length_b   19.935
_cell_length_c   11.753
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.20309  -0.25493   0.12805                    #  1
C2        0.16911  -0.19419   0.07556                    #  2
C3        0.06343  -0.17531   0.07254                    #  3
C4       -0.00852  -0.21963   0.12436                    #  4
C5        0.02164  -0.28134   0.17831                    #  5
C6        0.12757  -0.29776   0.17898                    #  6
N7        0.25053  -0.16278   0.03457                    #  7
O8        0.33780  -0.20744   0.06446                    #  8
N'9       0.30199  -0.26218   0.12106                    #  9
N'10      0.01964  -0.12222   0.02862                    # 10
O11      -0.08190  -0.12868   0.04890                    # 11
N12      -0.10040  -0.19265   0.11178                    # 12
N'13     -0.03347  -0.32718   0.22922                    # 13
O14       0.03225  -0.37546   0.26554                    # 14
N15       0.13802  -0.35614   0.23254                    # 15
O16      -0.18632  -0.20769   0.13797                    # 16
O17       0.26654  -0.11117  -0.01631                    # 17
O18       0.20794  -0.39271   0.25724                    # 18
C1a       0.18234   0.04688  -0.00076                    # 37
C2a       0.23538   0.09975  -0.05005                    # 38
C3a       0.27846   0.14963   0.01819                    # 39
C4a       0.27037   0.14600   0.13597                    # 40
C5a       0.21786   0.09267   0.18562                    # 41
C6a       0.17346   0.04346   0.11741                    # 42
H10a      0.14974   0.00896  -0.05580                     # 43
H11a      0.13241   0.00203   0.15580                     # 44
H12a      0.30455   0.18538   0.18671                     # 45
H13a      0.21125   0.09004   0.27751                     # 46
```

```
N7a       0.25113   0.09750  -0.17424                    # 57
O8a       0.17936   0.07779  -0.23212                    # 58
O9a       0.33586   0.11265  -0.20937                    # 59
N14a      0.32589   0.21027  -0.03030                    # 63
O15a      0.28450   0.23519  -0.11365                    # 64
O16a      0.40051   0.23263   0.01976                    # 65
C1a       0.58683   0.13998   0.12586                   # 69
C2a       0.56893   0.10990   0.02104                   # 70
C3a       0.50751   0.05285   0.01372                   # 71
C4a       0.46218   0.02659   0.11087                   # 72
C5a       0.47942   0.05705   0.21601                   # 73
C6a       0.54204   0.11337   0.22358                   # 74
H10a      0.63479   0.18414   0.12893                    # 75
H11a      0.55573   0.13705   0.30525                    # 76
H12a      0.41493  -0.01766   0.10259                    # 77
H13a      0.44434   0.03636   0.29182                    # 78
N7a       0.60973   0.14376  -0.08076                   # 89
O8a       0.69506   0.16831  -0.07244                   # 90
O9a       0.55361   0.14729  -0.16382                   # 91
N14a      0.49505   0.01502  -0.09322                    # 95
O15a      0.57062   0.00878  -0.15338                    # 96
O16a      0.41100  -0.00971  -0.11099                    # 97
C1a      -0.06593   0.11422  -0.08914                   #101
C2a      -0.06742   0.13287  -0.20310                   #102
C3a      -0.12432   0.09600  -0.28167                   #103
C4a      -0.18151   0.04123  -0.24604                   #104
C5a      -0.18075   0.02277  -0.13152                   #105
C6a      -0.12265   0.05893  -0.05339                   #106
H10a      -0.02111   0.14373  -0.03017                   #107
H11a      -0.12176   0.04459   0.03564                   #108
H12a      -0.22490   0.01361  -0.30886                   #109
H13a      -0.22508  -0.02014  -0.10389                   #110
N7a       -0.01439   0.19540  -0.23440                   #121
O8a        0.06751   0.20615  -0.18761                   #122
O9a       -0.05824   0.23302  -0.30072                   #123
N14a      -0.11977   0.10935  -0.40499                   #127
O15a      -0.03640   0.12380  -0.44477                   #128
O16a      -0.19905   0.10204  -0.45879                   #129
#END
```

```
data_ BTF-1,2-dinitrobenzene(2:1)_-7.20949E+01
_chemical_name_systematic
;RAS b3lyp-d3
```

E(total)=-7.20949E+01 E(coul)=-1.31887E+01 E(vdW)=-5.89061E+01 Density= 1.83958
;
_cell_length_a 11.642
_cell_length_b 6.925
_cell_length_c 15.164
_cell_angle_alpha 90.00
_cell_angle_beta 83.13
_cell_angle_gamma 90.00
_cell_formula_units_Z 2
_symmetry_space_group_name_H-M 'P 21 '
_symmetry_Int_Tables_number 4
loop_
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

C1	0.27764	-0.18024	0.14285	# 1
C2	0.35886	-0.13571	0.20359	# 2
C3	0.35402	0.04194	0.25322	# 3
C4	0.26414	0.17604	0.24017	# 4
C5	0.18021	0.13829	0.17986	# 5
C6	0.18887	-0.04033	0.13217	# 6
N7	0.43219	-0.28314	0.20300	# 7
O8	0.39218	-0.42315	0.13820	# 8
N'9	0.29795	-0.34887	0.10494	# 9
N'10	0.42056	0.10513	0.31086	# 10
O11	0.37865	0.28146	0.33840	# 11
N12	0.27591	0.32804	0.29197	# 12
N'13	0.09336	0.24374	0.16013	# 13
O14	0.04104	0.14168	0.09933	# 14
N15	0.10376	-0.04490	0.08096	# 15
O16	0.22595	0.47947	0.30742	# 16
O17	0.51541	-0.32259	0.24010	# 17
O18	0.07050	-0.15688	0.02841	# 18
C1	-0.23129	0.31321	0.21821	# 37
C2	-0.30465	0.35248	0.15114	# 38
C3	-0.29736	0.52985	0.10124	# 39
C4	-0.21321	0.66915	0.12065	# 40
C5	-0.13728	0.63680	0.18748	# 41
C6	-0.14806	0.45823	0.23515	# 42
N7	-0.37392	0.20092	0.14667	# 43
O8	-0.33969	0.06390	0.21501	# 44
N'9	-0.25254	0.14385	0.25518	# 45

```
N'10     -0.35703   0.58864   0.03831                          # 46
O11      -0.31596   0.76702   0.01334                          # 47
N12      -0.22149   0.81991   0.06742                          # 48
N'13     -0.05635   0.74736   0.21345                          # 49
O14      -0.01028   0.64893   0.27859                          # 50
N15      -0.07051   0.45902   0.29285                          # 51
O16      -0.17347   0.97397   0.05523                          # 52
O17      -0.45047   0.15638   0.10337                          # 53
O18      -0.04198   0.34951   0.34834                          # 54
C1a       0.36332   0.06558   0.57697                         # 73
C2a       0.30815  -0.05291   0.52115                         # 74
C3a       0.20842   0.01079   0.48710                         # 75
C4a       0.16504   0.19461   0.50733                         # 76
C5a       0.22087   0.31429   0.56278                         # 77
C6a       0.31936   0.24954   0.59791                         # 78
H10a      0.44045   0.01231   0.60238                          # 79
H11a      0.36276   0.34217   0.64118                          # 80
H12a      0.08761   0.24009   0.47996                          # 81
H13a      0.18667   0.45741   0.57881                          # 82
N7a       0.36442  -0.23794   0.49412                         # 93
O8a       0.40861  -0.32710   0.55140                         # 94
O9a       0.36707  -0.28387   0.41585                         # 95
N14a      0.13994  -0.11662   0.43553                          # 99
O15a      0.12893  -0.28507   0.45987                          #100
O16a      0.09520  -0.04163   0.37469                          #101
#END



data_ BTF-1,2-dinitrobenzene(3:1)_-9.55479E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-9.55479E+01 E(coul)=-2.39337E+01 E(vdW)=-7.16142E+01 Density= 1.77657
;
_cell_length_a   13.546
_cell_length_b   18.944
_cell_length_c    6.747
_cell_angle_alpha    90.00
_cell_angle_beta     86.54
_cell_angle_gamma    90.00
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P 21    '
_symmetry_Int_Tables_number   4
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
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 2 -x,1/2+y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1      -0.22747  -0.07136  -0.36919                    #  1
C2      -0.27372  -0.05857  -0.17632                    #  2
C3      -0.28972   0.01165  -0.09923                    #  3
C4      -0.25763   0.06967  -0.22255                    #  4
C5      -0.21071   0.05971  -0.41776                    #  5
C6      -0.19655  -0.01111  -0.48732                    #  6
N7      -0.29595  -0.12088  -0.09439                    #  7
O8      -0.26088  -0.17366  -0.24741                    #  8
N'9     -0.22033  -0.13892  -0.40929                    #  9
N'10    -0.33039   0.03264   0.07190                    # 10
O11     -0.32726   0.10449   0.07032                    # 11
N12     -0.27948   0.12882  -0.12308                    # 12
N'13    -0.17718   0.10629  -0.54880                    # 13
O14     -0.13976   0.06916  -0.70909                    # 14
N15     -0.15248  -0.00794  -0.66872                    # 15
O16     -0.26963   0.19134  -0.15386                    # 16
O17     -0.33448  -0.14126   0.06143                    # 17
O18     -0.12379  -0.05008  -0.79375                    # 18
C1       0.06408   0.29147   0.83081                   # 37
C2       0.05587   0.25779   0.64277                   # 38
C3      -0.03360   0.26028   0.53810                   # 39
C4      -0.11599   0.29805   0.62831                   # 40
C5      -0.11163   0.33287   0.81728                   # 41
C6      -0.02103   0.32878   0.91511                   # 42
N7       0.14207   0.22688   0.59362                   # 43
O8       0.20502   0.24315   0.76214                   # 44
N'9      0.15172   0.28256   0.89934                   # 45
N'10    -0.05365   0.23277   0.36688                    # 46
O11     -0.14885   0.25068   0.33579                    # 47
N12     -0.18980   0.29356   0.50749                    # 48
N'13    -0.17922   0.36929   0.91996                    # 49
O14     -0.13732   0.39079   1.08826                    # 50
N15     -0.03342   0.36419   1.08508                    # 51
O16     -0.27396   0.31476   0.50823                    # 52
O17      0.17610   0.19214   0.45563                    # 53
O18      0.01672   0.37772   1.22233                    # 54
C1       0.43461  -0.11772   0.11199                   # 73
C2       0.43996  -0.19202   0.07516                   # 74
C3       0.48209  -0.24038   0.21139                   # 75
C4       0.51934  -0.21186   0.38843                   # 76
C5       0.51575  -0.13752   0.43262                   # 77
```

```
C6       0.47315  -0.09174   0.29240                          # 78
N7       0.40062  -0.20415  -0.09755                          # 79
O8       0.37019  -0.13298  -0.16717                          # 80
N'9      0.39363  -0.08366  -0.03085                          # 81
N'10     0.49277  -0.30907   0.20107                          # 82
O11      0.53693  -0.32910   0.36822                          # 83
N12      0.55438  -0.26525   0.49129                          # 84
N'13     0.54606  -0.10289   0.58577                          # 85
O14      0.52534  -0.03354   0.55495                          # 86
N15      0.47745  -0.02622   0.36226                          # 87
O16      0.59319  -0.27191   0.64685                          # 88
O17      0.38608  -0.25537  -0.19851                          # 89
O18      0.45319   0.03165   0.30765                          # 90
C1a      0.14842   0.11406   0.03285                         #109
C2a      0.10398   0.08123  -0.12310                         #110
C3a      0.16140   0.04434  -0.26760                         #111
C4a      0.26312   0.03896  -0.25419                         #112
C5a      0.30775   0.07139  -0.09687                         #113
C6a      0.25062   0.10918   0.04564                         #114
H10a     0.10204   0.14231   0.14265                          #115
H11a     0.28517   0.13457   0.16784                          #116
H12a     0.30574   0.01000  -0.36835                          #117
H13a     0.38719   0.06740  -0.08701                          #118
N7a     -0.00499   0.08207  -0.11902                         #129
O8a     -0.04611   0.13709  -0.06447                         #130
O9a     -0.04597   0.02694  -0.16193                         #131
N14a     0.11929   0.01513  -0.44672                          #135
O15a     0.05660   0.05081  -0.52391                          #136
O16a     0.15356  -0.04117  -0.50921                          #137
#END
```

Simulated cocrystal structures of BTF-1,3-dinitrobenzene

```
data___ BTF-1,3-dinitrobenzene(1:1)____-4.51596E+01
_chemical_name_systematic
;RAS m-dnb-d3

E(total)=-4.51596E+01 E(coul)=-1.75047E+01 E(vdW)=-2.81362E+01 Density= 1.75265
;
_cell_length_a    7.417
_cell_length_b   17.617
_cell_length_c   12.200
_cell_angle_alpha    90.00
_cell_angle_beta     87.46
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
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_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       0.18026  -0.32365  -0.08362                    #  1
C2       0.13969  -0.38283  -0.00613                    #  2
C3      -0.03179  -0.38775   0.05354                    #  3
C4      -0.16377  -0.33086   0.03318                    #  4
C5      -0.12983  -0.27010  -0.04394                    #  5
C6       0.04271  -0.26782  -0.10107                    #  6
N7       0.28405  -0.42747  -0.00308                    #  7
O8       0.41791  -0.39278  -0.08335                    #  8
N'9      0.34350  -0.33003  -0.12834                    #  9
N'10    -0.09078  -0.43748   0.12655                    # 10
O11     -0.26209  -0.41628   0.15763                    # 11
N12     -0.31004  -0.34625   0.09631                    # 12
N'13    -0.23409  -0.21399  -0.07222                    # 13
O14     -0.13719  -0.17244  -0.14830                    # 14
N15      0.04462  -0.20779  -0.16725                    # 15
O16     -0.45755  -0.31823   0.11240                    # 16
O17      0.32454  -0.48411   0.04599                    # 17
O18      0.15164  -0.17916  -0.23241                    # 18
C1a      0.50994  -0.11500   0.14397                    # 37
C2a      0.36395  -0.07258   0.11098                    # 38
C3a      0.36114   0.00650   0.11524                    # 39
C4a      0.51034   0.04454   0.15404                    # 40
C5a      0.65933   0.00392   0.18788                    # 41
C6a      0.65613  -0.07510   0.18216                    # 42
H13a     0.50979  -0.17631   0.14010                    # 43
H14a     0.24370   0.03661   0.08844                    # 44
H15a     0.51049   0.10604   0.15792                    # 45
H16a     0.77692   0.03200   0.21834                    # 46
N7a      0.20576  -0.11318   0.06970                    # 59
O9a      0.08654  -0.07463   0.03037                    # 60
O10a     0.20425  -0.18269   0.07741                    # 61
N8a      0.81421  -0.11842   0.21802                    # 66
O11a     0.81336  -0.18745   0.20406                    # 67
O12a     0.93583  -0.08240   0.25935                    # 68
#END
```

```
data_ BTF-1,3-dinitrobenzene(1:2)_-6.77830E+01
_chemical_name_systematic
;RAS m-dnb-d3

E(total)=-6.77830E+01 E(coul)=-1.61926E+01 E(vdW)=-5.15904E+01 Density= 1.70270
;
_cell_length_a    9.025
_cell_length_b    9.056
_cell_length_c   14.264
_cell_angle_alpha    91.04
_cell_angle_beta     96.43
_cell_angle_gamma    97.59
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
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  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.09141   0.05695  -0.33534                      #  1
C2        0.06695   0.05676  -0.31234                      #  2
C3        0.12978   0.00136  -0.22475                      #  3
C4        0.02804  -0.05477  -0.15973                      #  4
C5       -0.13227  -0.05711  -0.17942                      #  5
C6       -0.18890  -0.00079  -0.26743                      #  6
N7        0.13471   0.11424  -0.38415                      #  7
O8        0.00937   0.15062  -0.45373                      #  8
N'9      -0.12387   0.11214  -0.41828                      #  9
N'10      0.27022  -0.00700  -0.19273                      # 10
O11       0.26840  -0.06815  -0.10626                      # 11
N12       0.10934  -0.09952  -0.08458                      # 12
N'13     -0.24025  -0.10394  -0.12849                      # 13
O14      -0.37168  -0.08127  -0.17951                      # 14
N15      -0.33795  -0.01352  -0.27077                      # 15
O16       0.08360  -0.15435  -0.01051                      # 16
O17       0.26287   0.14019  -0.40255                      # 17
O18      -0.44037   0.01537  -0.32644                      # 18
C1a       0.21781  -0.50809   0.00415                     # 37
C2a       0.26220  -0.40455   0.07843                     # 38
C3a       0.38034  -0.28919   0.07617                     # 39
```

```
C4a       0.45695  -0.27709  -0.00357                    # 40
C5a       0.41566  -0.37889  -0.07950                    # 41
C6a       0.29680  -0.49244  -0.07411                    # 42
H13a      0.12590  -0.59687   0.00712                     # 43
H14a      0.41003  -0.21172   0.13611                     # 44
H15a      0.54913  -0.18805  -0.00655                     # 45
H16a      0.47318  -0.37212  -0.14226                     # 46
N7a       0.18075  -0.41770   0.16284                    # 57
O9a       0.22209  -0.32482   0.22758                    # 58
O10a      0.07724  -0.52043   0.16275                     # 59
N8a       0.25273  -0.60054  -0.15447                    # 63
O11a      0.14765  -0.69929  -0.14765                     # 64
O12a      0.32428  -0.58437  -0.22285                     # 65
C1a       0.21798  -0.50579  -0.49445                    # 69
C2a       0.23353  -0.39527  -0.42379                    # 70
C3a       0.33731  -0.26655  -0.42271                    # 71
C4a       0.42902  -0.24782  -0.49521                    # 72
C5a       0.41668  -0.35629  -0.56734                    # 73
C6a       0.31131  -0.48321  -0.56550                    # 74
H13a      0.13687  -0.60493  -0.49416                     # 75
H14a      0.34451  -0.18414  -0.36586                     # 76
H15a      0.51037  -0.14839  -0.49551                     # 77
H16a      0.48644  -0.34462  -0.62447                     # 78
N7a       0.13614  -0.41548  -0.34704                    # 89
O9a       0.15202  -0.31622  -0.28539                    # 90
O10a      0.04586  -0.52997  -0.34992                     # 91
N8a       0.29793  -0.59840  -0.64185                    # 95
O11a      0.20413  -0.70891  -0.63830                     # 96
O12a      0.38168  -0.57588  -0.70387                     # 97
#END


data_ BTF-1,3-dinitrobenzene(1:3)_-8.51619E+01
_chemical_name_systematic
;RAS m-dnb-d3

E(total)=-8.51619E+01 E(coul)=-1.86548E+01 E(vdW)=-6.65072E+01 Density= 1.65493
;
_cell_length_a   11.880
_cell_length_b   20.707
_cell_length_c    6.197
_cell_angle_alpha    90.00
_cell_angle_beta     84.78
_cell_angle_gamma    90.00
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P 21    '
_symmetry_Int_Tables_number   4
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_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       0.74589   0.48591   0.04567                    #  1
C2       0.74733   0.52380   0.23839                    #  2
C3       0.65863   0.56881   0.30577                    #  3
C4       0.56693   0.57496   0.17274                    #  4
C5       0.56138   0.53797  -0.02276                    #  5
C6       0.65165   0.49394  -0.08245                    #  6
N7       0.84084   0.50882   0.33029                    #  7
O8       0.89815   0.45920   0.18369                    #  8
N'9      0.83459   0.44826   0.01521                    #  9
N'10     0.64669   0.60685   0.47534                    # 10
O11      0.54800   0.63956   0.46311                    # 11
N12      0.49561   0.61861   0.26436                    # 12
N'13     0.48462   0.53759  -0.16187                    # 13
O14      0.51975   0.49394  -0.31812                    # 14
N15      0.62946   0.46527  -0.26596                    # 15
O16      0.40685   0.64218   0.22404                    # 16
O17      0.88412   0.52534   0.49053                    # 17
O18      0.67494   0.42518  -0.38589                    # 18
C1a     -0.19359   0.04182  -0.20316                    # 37
C2a     -0.23672  -0.00718  -0.06636                    # 38
C3a     -0.19411  -0.02052   0.13118                    # 39
C4a     -0.10486   0.01666   0.19410                    # 40
C5a     -0.05935   0.06625   0.06114                    # 41
C6a     -0.10468   0.07784  -0.13499                    # 42
H13a    -0.22769   0.05149  -0.35583                    # 43
H14a    -0.23104  -0.05930   0.23122                    # 44
H15a    -0.07065   0.00696   0.34722                    # 45
H16a     0.00994   0.09585   0.10598                    # 46
N7a     -0.33133  -0.04650  -0.13355                    # 57
O9a     -0.36801  -0.08954  -0.00984                    # 58
O10a    -0.36704  -0.03361  -0.30836                    # 59
N8a     -0.05664   0.13036  -0.27631                    # 63
O11a    -0.09833   0.13941  -0.44800                    # 64
O12a     0.02192   0.16152  -0.21249                    # 65
C1a      0.38133   0.25570   0.17870                    # 69
C2a      0.28594   0.23301   0.30206                    # 70
C3a      0.25565   0.25422   0.51289                    # 71
C4a      0.32353   0.29992   0.60362                    # 72
```

```
C5a       0.41991   0.32381   0.48484                    # 73
C6a       0.44690   0.30120   0.27457                    # 74
H13a      0.40354   0.23871   0.01539                     # 75
H14a      0.18038   0.23486   0.60143                     # 76
H15a      0.30126   0.31696   0.76741                     # 77
H16a      0.47411   0.35930   0.55127                     # 78
N7a       0.21418   0.18458   0.20539                    # 89
O9a       0.13030   0.16526   0.31768                    # 90
O10a      0.24303   0.16684   0.01944                     # 91
N8a       0.54900   0.32643   0.14822                    # 95
O11a      0.57056   0.30561  -0.03648                     # 96
O12a      0.60559   0.36663   0.23652                     # 97
C1a      -0.08585   0.28333  -0.75691                    #101
C2a      -0.18742   0.25870  -0.66222                    #102
C3a      -0.22984   0.27421  -0.45142                    #103
C4a      -0.16813   0.31600  -0.33085                    #104
C5a      -0.06585   0.34168  -0.42035                    #105
C6a      -0.02673   0.32481  -0.63177                    #106
H13a      -0.05423   0.27077  -0.92065                     #107
H14a      -0.30948   0.25357  -0.38598                     #108
H15a      -0.19985   0.32859  -0.16662                     #109
H16a      -0.01622   0.37423  -0.33041                     #110
N7a      -0.25262   0.21441  -0.79048                    #121
O9a      -0.34217   0.19327  -0.70320                    #122
O10a      -0.21310   0.20166  -0.97560                     #123
N8a       0.08166   0.35195  -0.72714                    #127
O11a      0.11391   0.33620  -0.91364                     #128
O12a      0.13236   0.38851  -0.61329                     #129
#END



data_ BTF-1,3-dinitrobenzene(2:1)_-7.25939E+01
_chemical_name_systematic
;RAS m-dnb-d3

E(total)=-7.25939E+01 E(coul)=-1.65524E+01 E(vdW)=-5.60415E+01 Density= 1.80730
;
_cell_length_a    7.084
_cell_length_b   18.464
_cell_length_c   18.907
_cell_angle_alpha    90.00
_cell_angle_beta     92.29
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
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_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1      0.76231   0.61102   0.24968                    #  1
C2      0.78731   0.64193   0.18132                    #  2
C3      0.64317   0.63826   0.12555                    #  3
C4      0.47043   0.60221   0.14032                    #  4
C5      0.43806   0.57019   0.20821                    #  5
C6      0.58579   0.57533   0.26180                    #  6
N7      0.95833   0.67173   0.18188                    #  7
O8      1.03943   0.65769   0.25475                    #  8
N'9     0.91079   0.62056   0.29226                    #  9
N'10    0.64252   0.66331   0.06068                    # 10
O11     0.47193   0.64535   0.02979                    # 11
N12     0.35889   0.60522   0.08210                    # 12
N'13    0.29022   0.53559   0.23051                    # 13
O14     0.33217   0.51642   0.29890                    # 14
N15     0.52630   0.54252   0.31945                    # 15
O16     0.20204   0.58440   0.06480                    # 16
O17     1.05125   0.70426   0.14008                    # 17
O18     0.59024   0.53082   0.37856                    # 18
C1     -0.04018   0.28720   0.07039                    # 37
C2     -0.17881   0.23512   0.08936                    # 38
C3     -0.35226   0.25567   0.12111                    # 39
C4     -0.38367   0.33105   0.13356                    # 40
C5     -0.24877   0.38566   0.11547                    # 41
C6     -0.07873   0.36236   0.08405                    # 42
N7     -0.11486   0.16994   0.07226                    # 43
O8      0.07243   0.18417   0.04139                    # 44
N'9     0.10633   0.25678   0.04235                    # 45
N'10   -0.49275   0.21559   0.14152                    # 46
O11    -0.62210   0.26175   0.16808                    # 47
N12    -0.55046   0.33758   0.16285                    # 48
N'13   -0.25480   0.45616   0.12310                    # 49
O14    -0.09155   0.48261   0.09749                    # 50
N15     0.02410   0.42100   0.07185                    # 51
O16    -0.64540   0.38692   0.18379                    # 52
O17    -0.17116   0.10835   0.07619                    # 53
O18     0.17535   0.43326   0.04698                    # 54
```

```
C1a       0.25213   0.15775  -0.16034                    # 73
C2a       0.08734   0.11766  -0.15471                    # 74
C3a       0.06171   0.06870  -0.09979                    # 75
C4a       0.20676   0.05954  -0.04852                    # 76
C5a       0.37417   0.09880  -0.05238                    # 77
C6a       0.39351   0.14716  -0.10827                    # 78
H13a      0.26957   0.19549  -0.20331                     # 79
H14a     -0.06970   0.03893  -0.09808                     # 80
H15a      0.18927   0.02169  -0.00542                     # 81
H16a      0.48903   0.09276  -0.01331                     # 82
N7a      -0.06612   0.12750  -0.20915                    # 93
O9a      -0.21043   0.09145  -0.20302                    # 94
O10a     -0.03939   0.17100  -0.25686                     # 95
N8a       0.57078   0.18886  -0.11252                    # 99
O11a      0.58364   0.23102  -0.16234                     #100
O12a      0.69367   0.17855  -0.06586                     #101
#END



data_ BTF-1,3-dinitrobenzene(3:1)_-9.68200E+01
_chemical_name_systematic
;RAS m-dnb-d3

E(total)=-9.68200E+01 E(coul)=-2.18265E+01 E(vdW)=-7.49935E+01 Density= 1.80997
;
_cell_length_a    6.854
_cell_length_b   11.885
_cell_length_c   10.467
_cell_angle_alpha    89.55
_cell_angle_beta     95.52
_cell_angle_gamma    92.10
_cell_formula_units_Z  1
_symmetry_space_group_name_H-M 'P 1     '
_symmetry_Int_Tables_number   1
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.26776   0.48182   0.01351                    #  1
C2        0.36757   0.39859  -0.05064                    #  2
C3        0.55129   0.42315  -0.10289                    #  3
C4        0.63375   0.53519  -0.08893                    #  4
```

C5	0.53932	0.62208	-0.02522	# 5
C6	0.35706	0.59329	0.02497	# 6
N7	0.26028	0.30304	-0.05020	# 7
O8	0.08691	0.33122	0.01813	# 8
N'9	0.10360	0.44147	0.05338	# 9
N'10	0.66115	0.35786	-0.16375	# 10
O11	0.81932	0.42247	-0.19264	# 11
N12	0.80133	0.53894	-0.14350	# 12
N'13	0.59362	0.72773	-0.00423	# 13
O14	0.45214	0.77337	0.05991	# 14
N15	0.29675	0.68507	0.07910	# 15
O16	0.92805	0.60958	-0.15965	# 16
O17	0.27305	0.20851	-0.08947	# 17
O18	0.15727	0.70897	0.13452	# 18
C1	-0.01051	-0.63757	0.50439	# 37
C2	-0.13078	-0.72798	0.54832	# 38
C3	-0.32935	-0.74999	0.49382	# 39
C4	-0.40550	-0.67782	0.39244	# 40
C5	-0.29066	-0.58567	0.34467	# 41
C6	-0.09424	-0.56743	0.40212	# 42
N7	-0.02526	-0.78108	0.64198	# 43
O8	0.16871	-0.71860	0.65431	# 44
N'9	0.16455	-0.63286	0.56711	# 45
N'10	-0.45836	-0.82811	0.52212	# 46
O11	-0.62373	-0.81176	0.44210	# 47
N12	-0.58902	-0.71305	0.35692	# 48
N'13	-0.33671	-0.51226	0.25365	# 49
O14	-0.17550	-0.44287	0.24647	# 50
N15	-0.01624	-0.47910	0.34398	# 51
O16	-0.71908	-0.68461	0.27844	# 52
O17	-0.05143	-0.86079	0.71147	# 53
O18	0.13998	-0.42784	0.35297	# 54
C1	0.39523	-0.09716	0.37631	# 73
C2	0.53906	-0.18175	0.38951	# 74
C3	0.52545	-0.27557	0.47647	# 75
C4	0.36119	-0.28249	0.55110	# 76
C5	0.21235	-0.19962	0.54148	# 77
C6	0.23279	-0.10809	0.45365	# 78
N7	0.67415	-0.15525	0.31011	# 79
O8	0.60659	-0.04884	0.24615	# 80
N'9	0.43621	-0.01975	0.29212	# 81
N'10	0.64254	-0.35951	0.50028	# 82
O11	0.56277	-0.42515	0.59046	# 83
N12	0.37797	-0.37456	0.62384	# 84
N'13	0.05428	-0.19308	0.60185	# 85
O14	-0.03632	-0.09836	0.55764	# 86
N15	0.08092	-0.04253	0.46030	# 87

```
O16       0.28451  -0.42056   0.70274                          # 88
O17       0.82389  -0.19529   0.28224                          # 89
O18       0.02464   0.04351   0.40927                          # 90
C1a      -0.30607   0.04401  -0.03342                          #109
C2a      -0.24338  -0.04135  -0.10796                          #110
C3a      -0.05311  -0.08024  -0.09126                          #111
C4a       0.07946  -0.03175   0.00378                         #112
C5a       0.02194   0.05410   0.08048                         #113
C6a      -0.16985   0.09029   0.06032                         #114
H13a     -0.45424   0.07313  -0.04772                          #115
H14a     -0.01238  -0.14700  -0.15216                          #116
H15a      0.22806  -0.06095   0.01812                          #117
H16a      0.12181   0.09323   0.15494                          #118
N7a      -0.38427  -0.09257  -0.20862                          #129
O9a      -0.32536  -0.16789  -0.27327                          #130
O10a     -0.55075  -0.05655  -0.22103                          #131
N8a      -0.23131   0.18127   0.14145                         #135
O11a     -0.40111   0.21133   0.12141                          #136
O12a     -0.10822   0.22083   0.22366                          #137
#END
```

Simulated cocrystal structures of BTF-1,4-dinitrobenzene

```
data_ BTF-1,4-dinitrobenzene(1:1)_-3.61177E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-3.61177E+01 E(coul)=-6.22070E+00 E(vdW)=-3.07641E+01 Density= 1.79845
;
_cell_length_a    8.330
_cell_length_b    8.886
_cell_length_c   11.275
_cell_angle_alpha    71.05
_cell_angle_beta     81.46
_cell_angle_gamma    81.40
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
```

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_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1      0.26635  -1.38092   0.52076                    #  1
C2      0.34358  -1.31531   0.59510                    #  2
C3      0.32912  -1.14599   0.57690                    #  3
C4      0.23365  -1.04241   0.48065                    #  4
C5      0.15341  -1.10226   0.40321                    #  5
C6      0.17165  -1.27144   0.42513                    #  6
N7      0.42355  -1.43636   0.67654                    #  7
O8      0.39196  -1.58211   0.64893                    #  8
N'9     0.29549  -1.53723   0.55308                    #  9
N'10    0.39092  -1.06659   0.63577                    # 10
O11     0.34019  -0.90895   0.58220                    # 11
N12     0.23689  -0.89306   0.48031                    # 12
N'13    0.06247  -1.02535   0.31203                    # 13
O14     0.01673  -1.13811   0.26975                    # 14
N15     0.08844  -1.29975   0.34403                    # 15
O16     0.17962  -0.76162   0.42093                    # 16
O17     0.50732  -1.45087   0.75920                    # 17
O18     0.06195  -1.41668   0.32075                    # 18
C1a     0.61354  -0.29226  -0.02773                    # 37
C2a     0.60568  -0.20933   0.05915                    # 38
C3a     0.74313  -0.15905   0.08574                    # 39
C4a     0.89422  -0.19300   0.02306                    # 40
C5a     0.90208  -0.27593  -0.06383                    # 41
C6a     0.76463  -0.32621  -0.09042                    # 42
H10a    0.50304  -0.32859  -0.04489                    # 43
H11a    0.73027  -0.09501   0.15408                    # 44
H15a    0.77749  -0.39025  -0.15876                    # 45
H16a    1.00472  -0.15667   0.04022                    # 46
N7a     0.44455  -0.17318   0.12611                    # 59
O8a     0.32552  -0.22059   0.10232                    # 60
O9a     0.44069  -0.09818   0.20103                    # 61
N12a    1.06321  -0.31186  -0.13080                    # 66
O13a    1.07274  -0.40880  -0.18898                    # 67
O14a    1.17661  -0.24221  -0.12382                    # 68
#END



data_ BTF-1,4-dinitrobenzene(1:2)_-6.74377E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-6.74377E+01 E(coul)=-1.36784E+01 E(vdW)=-5.37593E+01 Density= 1.72619
```

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_cell_length_a   33.658
_cell_length_b    5.352
_cell_length_c   12.717
_cell_angle_alpha    90.00
_cell_angle_beta     98.78
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.40737   0.23214  -0.10446                    #  1
C2        0.43565   0.03468  -0.07648                    #  2
C3        0.43178  -0.14045   0.00731                    #  3
C4        0.39828  -0.11203   0.06326                    #  4
C5        0.36896   0.08342   0.03826                    #  5
C6        0.37419   0.25246  -0.04567                    #  6
N7        0.46344   0.05092  -0.14015                    #  7
O8        0.45094   0.27058  -0.20989                    #  8
N9        0.41661   0.36911  -0.18267                    #  9
N10       0.45463  -0.32990   0.04290                    # 10
O11       0.43763  -0.43463   0.12292                    # 11
N12       0.40062  -0.29153   0.13630                    # 12
N13       0.33687   0.13590   0.08089                    # 13
O14       0.31954   0.33916   0.02808                    # 14
N15       0.34405   0.41573  -0.05504                    # 15
O16       0.38107  -0.35543   0.20384                    # 16
O17       0.49344  -0.06322  -0.15179                    # 17
O18       0.33360   0.59376  -0.11093                    # 18
C1a       0.23177   0.42613  -0.38884                    # 37
C2a       0.20511   0.31957  -0.32793                    # 38
C3a       0.20063   0.40843  -0.22739                    # 39
C4a       0.22369   0.61163  -0.18619                    # 40
C5a       0.25035   0.71819  -0.24710                    # 41
C6a       0.25483   0.62933  -0.34764                    # 42
H10a      0.23409   0.34985  -0.46648                    # 43
H11a      0.17949   0.31882  -0.18338                    # 44
```

```
H15a      0.27597   0.71895  -0.39164                    # 45
H16a      0.22137   0.68791  -0.10854                    # 46
N7a       0.18059   0.10345  -0.37175                    # 57
O8a       0.18509   0.02866  -0.46053                    # 58
O9a       0.15731   0.01287  -0.31651                    # 59
N12a      0.27487   0.93431  -0.20328                    # 63
O13a      0.29815   1.02490  -0.25852                    # 64
O14a      0.27037   1.00911  -0.11450                    # 65
C1a       0.08030   0.39926  -0.19804                    # 69
C2a       0.05302   0.29830  -0.13755                    # 70
C3a       0.04853   0.39032  -0.03751                    # 71
C4a       0.07223   0.59098   0.00360                    # 72
C5a       0.09951   0.69194  -0.05690                    # 73
C6a       0.10400   0.59992  -0.15693                    # 74
H10a      0.08260   0.32072  -0.27530                    # 75
H11a      0.02689   0.30504   0.00618                    # 76
H15a      0.12564   0.68520  -0.20063                    # 77
H16a      0.06993   0.66953   0.08086                    # 78
N7a       0.02782   0.08487  -0.18127                    # 89
O8a       0.03235   0.00720  -0.26960                    # 90
O9a       0.00401  -0.00078  -0.12640                    # 91
N12a      0.12471   0.90537  -0.01317                    # 95
O13a      0.14852   0.99102  -0.06804                    # 96
O14a      0.12018   0.98304   0.07516                    # 97
#END



data_ BTF-1,4-dinitrobenzene(1:3)_-9.02460E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-9.02460E+01 E(coul)=-1.81237E+01 E(vdW)=-7.21223E+01 Density= 1.71598
;
_cell_length_a    8.166
_cell_length_b    8.688
_cell_length_c   21.324
_cell_angle_alpha    78.79
_cell_angle_beta     94.69
_cell_angle_gamma    98.92
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
```

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loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1      0.26541  0.37892  0.49056                 #  1
C2      0.34613  0.30006  0.45158                 #  2
C3      0.33112  0.12993  0.46091                 #  3
C4      0.23143  0.03938  0.51115                 #  4
C5      0.14756  0.11285  0.55174                 #  5
C6      0.16653  0.28225  0.54048                 #  6
N7      0.42962  0.41081  0.40911                 #  7
O8      0.39653  0.56415  0.42373                 #  8
N9      0.29576  0.53352  0.47384                 #  9
N10     0.39574  0.03942  0.43001                 # 10
O11     0.34283 -0.11316  0.45786                 # 11
N12     0.23490 -0.11319  0.51115                 # 12
N13     0.05258  0.04875  0.59936                 # 13
O14     0.00473  0.17070  0.62162                 # 14
N15     0.07957  0.32407  0.58295                 # 15
O16     0.17513 -0.23807  0.54207                 # 16
O17     0.51714  0.41250  0.36587                 # 17
O18     0.05182  0.44726  0.59527                 # 18
C1a     0.78044  0.06432  0.19378                 # 37
C2a     0.63818  0.12141  0.20602                 # 38
C3a     0.63834  0.21945  0.25058                 # 39
C4a     0.78642  0.26202  0.28418                 # 40
C5a     0.92868  0.20493  0.27194                 # 41
C6a     0.92852  0.10689  0.22738                 # 42
H10a    0.77353 -0.01151  0.15866                 # 43
H11a    0.52435  0.26051  0.25826                 # 44
H15a    1.04251  0.06583  0.21970                 # 45
H16a    0.79333  0.33785  0.31930                 # 46
N7a     0.48067  0.07613  0.17028                 # 57
O8a     0.48379 -0.01039  0.13127                 # 58
O9a     0.35703  0.12800  0.18193                 # 59
N12a    1.08619  0.25021  0.30768                 # 63
O13a    1.20983  0.19834  0.29603                 # 64
O14a    1.08307  0.33673  0.34669                 # 65
C1a     0.12926 -0.28164  0.24991                 # 69
C2a     0.13487 -0.38067  0.20619                 # 70
C3a     0.28118 -0.43134  0.19427                 # 71
C4a     0.42748 -0.38106  0.22733                 # 72
C5a     0.42187 -0.28203  0.27105                 # 73
C6a     0.27556 -0.23136  0.28297                 # 74
H10a    0.01230 -0.24577  0.25738                 # 75
H11a    0.27870 -0.50827  0.15982                 # 76
```

```
H15a      0.27804  -0.15443   0.31742                          # 77
H16a      0.54444  -0.41693   0.21986                          # 78
N7a      -0.02074  -0.43415   0.17103                         # 89
O8a      -0.14804  -0.38784   0.18240                         # 90
O9a      -0.01252  -0.52138   0.13276                         # 91
N12a      0.57748  -0.22855   0.30621                          # 95
O13a      0.56926  -0.14132   0.34448                          # 96
O14a      0.70478  -0.27486   0.29484                          # 97
C1a       0.19220   0.38025   0.01473                         #101
C2a       0.30359   0.39518  -0.03297                         #102
C3a       0.36203   0.26529  -0.04824                         #103
C4a       0.30698   0.11473  -0.01451                         #104
C5a       0.19559   0.09980   0.03319                         #105
C6a       0.13715   0.22969   0.04846                         #106
H10a      0.15070   0.48503   0.02469                          #107
H11a      0.44849   0.28345  -0.08573                          #108
H15a      0.05069   0.21153   0.08595                          #109
H16a      0.34848   0.00995  -0.02447                          #110
N7a       0.36215   0.55532  -0.06884                         #121
O8a       0.30881   0.66787  -0.05448                         #122
O9a       0.46031   0.56532  -0.11065                         #123
N12a      0.13703  -0.06034   0.06906                          #127
O13a      0.03887  -0.07034   0.11087                          #128
O14a      0.19037  -0.17289   0.05470                          #129
#END



data_ BTF-1,4-dinitrobenzene(2:1)_-7.26160E+01
_chemical_name_systematic
;RAS b3lyp-d3

E(total)=-7.26160E+01 E(coul)=-1.55251E+01 E(vdW)=-5.70909E+01 Density= 1.81641
;
_cell_length_a    6.202
_cell_length_b   33.266
_cell_length_c   12.747
_cell_angle_alpha    90.00
_cell_angle_beta     69.20
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
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 3 -x,-y,-z
 4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1      0.19396  0.19731  0.54591                    #  1
C2      0.34468  0.19737  0.60871                    #  2
C3      0.36920  0.23186  0.67178                    #  3
C4      0.23650  0.26688  0.67026                    #  4
C5      0.08231  0.26840  0.60844                    #  5
C6      0.06429  0.23332  0.54718                    #  6
N7      0.44588  0.16152  0.59586                    #  7
O8      0.34969  0.13890  0.52117                    #  8
N9      0.19824  0.16293  0.49500                    #  9
N10     0.49763  0.23702  0.73312                    # 10
O11     0.45691  0.27513  0.77459                    # 11
N12     0.28539  0.29474  0.73330                    # 12
N13    -0.05041  0.29762  0.59802                    # 13
O14    -0.16114  0.28354  0.53038                    # 14
N15    -0.08581  0.24131  0.49698                    # 15
O16     0.22591  0.32891  0.76094                    # 16
O17     0.58450  0.14531  0.62867                    # 17
O18    -0.16494  0.22334  0.43653                    # 18
C1      0.87601  0.09572 -0.20423                    # 37
C2      0.80661  0.05446 -0.19303                    # 38
C3      0.57083  0.04241 -0.13594                    # 39
C4      0.40362  0.07330 -0.08958                    # 40
C5      0.46432  0.11527 -0.09850                    # 41
C6      0.70092  0.12563 -0.15606                    # 42
N7      0.99364  0.03231 -0.24304                    # 43
O8      1.18493  0.06214 -0.28638                    # 44
N9      1.09786  0.09987 -0.25903                    # 45
N10     0.47845  0.00645 -0.11821                    # 46
O11     0.24904  0.01170 -0.06013                    # 47
N12     0.19989  0.05561 -0.04133                    # 48
N13     0.33485  0.14707 -0.06144                    # 49
O14     0.47719  0.17956 -0.09216                    # 50
N15     0.71763  0.16548 -0.15431                    # 51
O16     0.00464  0.06660  0.00907                    # 52
O17     1.03573 -0.00312 -0.25882                    # 53
O18     0.87079  0.18992 -0.18893                    # 54
C1a     0.84756  0.09948  0.35882                    # 73
C2a     0.71567  0.07127  0.43580                    # 74
C3a     0.52208  0.05291  0.42561                    # 75
C4a     0.45793  0.06315  0.33499                    # 76
```

```
C5a      0.58981   0.09135   0.25801                    # 77
C6a      0.78340   0.10972   0.26819                    # 78
H10a     0.99637   0.11285   0.37065                    # 79
H11a     0.42565   0.03119   0.48778                    # 80
H15a     0.87983   0.13144   0.20603                    # 81
H16a     0.30912   0.04978   0.32315                    # 82
N7a      0.78391   0.06039   0.53219                    # 93
O8a      0.95519   0.07699   0.53928                    # 94
O9a      0.66485   0.03545   0.59886                    # 95
N12a     0.52158   0.10224   0.16161                    # 99
O13a     0.64064   0.12718   0.09494                    #100
O14a     0.35030   0.08563   0.15453                    #101
#END
```

```
data_ BTF-1,4-dinitrobenzene(3:1)_-1.0047251E+02
_chemical_name_systematic
;RAS

E(total)=-9.89964E+01 E(coul)=-2.15212E+01 E(vdW)=-7.74751E+01 Density= 1.84462
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_cell_length_a   12.231
_cell_length_b   12.682
_cell_length_c   12.779
_cell_angle_alpha    71.69
_cell_angle_beta     63.62
_cell_angle_gamma    89.77
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       0.19620  -0.01867  -0.29282                    #  1
C2       0.10077  -0.11451  -0.21645                    #  2
C3       0.12503  -0.22359  -0.16086                    #  3
C4       0.24952  -0.23429  -0.18418                    #  4
C5       0.34896  -0.14054  -0.26033                    #  5
C6       0.31991  -0.03400  -0.31336                    #  6
```

N7	-0.00471	-0.08157	-0.21011	# 7
O8	0.03014	0.04082	-0.28711	# 8
N'9	0.15382	0.07182	-0.33369	# 9
N'10	0.04960	-0.31911	-0.08939	# 10
O11	0.11937	-0.39656	-0.06230	# 11
N12	0.25067	-0.34086	-0.12456	# 12
N'13	0.46677	-0.13551	-0.29092	# 13
O14	0.52069	-0.02706	-0.36459	# 14
N15	0.42423	0.03962	-0.37933	# 15
O16	0.32779	-0.39575	-0.11188	# 16
O17	-0.11125	-0.12560	-0.16025	# 17
O18	0.45365	0.13855	-0.44187	# 18
C1	0.30128	-0.14946	0.11420	# 37
C2	0.30728	-0.04768	0.13876	# 38
C3	0.25896	-0.04606	0.26347	# 39
C4	0.20355	-0.15086	0.36461	# 40
C5	0.19516	-0.25568	0.34502	# 41
C6	0.24457	-0.25266	0.21932	# 42
N7	0.36260	0.03621	0.02963	# 43
O8	0.39105	-0.01897	-0.06509	# 44
N'9	0.35060	-0.13168	-0.00546	# 45
N'10	0.25677	0.03847	0.30228	# 46
O11	0.20066	-0.00554	0.42908	# 47
N12	0.16571	-0.12990	0.47003	# 48
N'13	0.14804	-0.35799	0.42588	# 49
O14	0.16369	-0.42669	0.35871	# 50
N15	0.22710	-0.35751	0.22304	# 51
O16	0.11446	-0.18488	0.58005	# 52
O17	0.39136	0.13687	-0.00474	# 53
O18	0.24958	-0.40318	0.14738	# 54
C1	0.14445	-0.60043	-0.23827	# 73
C2	0.26160	-0.52872	-0.30439	# 74
C3	0.37466	-0.57176	-0.31910	# 75
C4	0.36712	-0.69054	-0.26490	# 76
C5	0.25159	-0.76641	-0.19744	# 77
C6	0.14198	-0.71934	-0.18551	# 78
N7	0.24244	-0.42364	-0.34467	# 79
O8	0.10611	-0.43358	-0.29989	# 80
N'9	0.05406	-0.54385	-0.23620	# 81
N'10	0.48841	-0.51876	-0.37603	# 82
O11	0.56067	-0.59861	-0.36253	# 83
N12	0.48101	-0.71144	-0.28954	# 84
N'13	0.22823	-0.87600	-0.14257	# 85
O14	0.10391	-0.90641	-0.09238	# 86
N15	0.04726	-0.80353	-0.12058	# 87
O16	0.52800	-0.79399	-0.26737	# 88
O17	0.30583	-0.33187	-0.40362	# 89

```
O18      -0.06313  -0.81273  -0.08381                    # 90
C1a      -0.36733   0.65753  -0.27971                   #109
C2a      -0.24365   0.66832  -0.36548                   #110
C3a      -0.14806   0.66840  -0.33419                   #111
C4a      -0.17727   0.65727  -0.21249                   #112
C5a      -0.30095   0.64648  -0.12672                   #113
C6a      -0.39654   0.64640  -0.15801                   #114
N7a      -0.21259   0.68016  -0.49493                   #115
O8a      -0.29850   0.67984  -0.52016                   #116
O9a      -0.10291   0.68954  -0.56876                   #117
H10a     -0.43801   0.65797  -0.30887                    #118
H11a     -0.05354   0.67705  -0.40441                    #119
N12a     -0.33201   0.63464   0.00273                    #120
O13a     -0.44169   0.62526   0.07656                    #121
O14a     -0.24610   0.63496   0.02796                    #122
H15a     -0.49106   0.63775  -0.08779                    #123
H16a     -0.10659   0.65683  -0.18333                    #124
#END
```

Simulated cocrystal structures of BTF-1,3,5-trinitrobenzene

```
data_ BTF-1,3,5-trinitrobenzene(1:1)_____-3.98822E+01
_chemical_name_systematic
;RAS tnb-d3

E(total)=-3.98822E+01 E(coul)=-1.38601E+01 E(vdW)=-2.65282E+01 Density= 1.83247
;
_cell_length_a    9.954
_cell_length_b   11.803
_cell_length_c   14.641
_cell_angle_alpha    90.00
_cell_angle_beta    101.37
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
```

_atom_site_fract_z

C1	0.67623	0.16889	0.75618	# 1
C2	0.60932	0.06496	0.77035	# 2
C3	0.50491	0.01556	0.69942	# 3
C4	0.46870	0.07402	0.61247	# 4
C5	0.53287	0.17886	0.59462	# 5
C6	0.63598	0.22433	0.66740	# 6
N7	0.66173	0.02898	0.85608	# 7
O8	0.76568	0.11659	0.89499	# 8
N'9	0.76758	0.19834	0.82960	# 9
N'10	0.43404	-0.07783	0.70065	# 10
O11	0.34873	-0.08566	0.61587	# 11
N12	0.37150	0.01407	0.55795	# 12
N'13	0.51239	0.24280	0.51997	# 13
O14	0.59960	0.33238	0.53936	# 14
N15	0.68078	0.32026	0.63619	# 15
O16	0.30515	0.02287	0.47973	# 16
O17	0.64432	-0.05128	0.90366	# 17
O18	0.76454	0.39172	0.66683	# 18
C1a	-0.01044	0.13055	0.42478	# 37
C2a	0.03177	0.08564	0.34725	# 38
C3a	0.13179	0.13660	0.30689	# 39
C4a	0.19013	0.23631	0.34711	# 40
C5a	0.15213	0.28521	0.42464	# 41
C6a	0.05158	0.23041	0.46196	# 42
H16a	-0.08846	0.08941	0.45500	# 43
H17a	0.16300	0.10011	0.24657	# 44
H18a	0.19894	0.36284	0.45475	# 45
N7a	-0.03215	-0.02048	0.30620	# 58
O10a	-0.12487	-0.06019	0.34046	# 59
O11a	0.01222	-0.06114	0.24091	# 60
N8a	0.29686	0.29240	0.30588	# 65
O14a	0.35029	0.37768	0.34514	# 66
O15a	0.32429	0.24953	0.23542	# 67
N9a	0.00872	0.28014	0.54434	# 72
O12a	0.06260	0.36978	0.57419	# 73
O13a	-0.07768	0.22805	0.57686	# 74

#END

data_ BTF-1,3,5-trinitrobenzene(1:2)_-7.04510E+01
_chemical_name_systematic
;RAS tnb-d3

E(total)=-7.04510E+01 E(coul)=-1.81465E+01 E(vdW)=-5.23045E+01 Density= 1.72065
;
_cell_length_a 9.912
_cell_length_b 18.975
_cell_length_c 15.939
_cell_angle_alpha 90.00
_cell_angle_beta 60.87
_cell_angle_gamma 90.00
_cell_formula_units_Z 4
_symmetry_space_group_name_H-M 'P 21/C '
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_as_xyz
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2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
loop_
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

C1	0.59417	0.12486	-0.09211	# 1
C2	0.59509	0.08696	-0.01482	# 2
C3	0.50983	0.11049	0.08331	# 3
C4	0.42216	0.17406	0.10227	# 4
C5	0.41730	0.21420	0.02713	# 5
C6	0.50405	0.18853	-0.06912	# 6
N7	0.68460	0.03060	-0.05196	# 7
O8	0.73994	0.03535	-0.15731	# 8
N'9	0.67935	0.09417	-0.17522	# 9
N'10	0.49797	0.08259	0.16185	# 10
O11	0.40331	0.12566	0.23554	# 11
N12	0.35351	0.18574	0.19642	# 12
N'13	0.34398	0.27279	0.03170	# 13
O14	0.37806	0.28854	-0.05990	# 14
N15	0.48320	0.23320	-0.12613	# 15
O16	0.26844	0.23015	0.25076	# 16
O17	0.72574	-0.01827	-0.02124	# 17
O18	0.52712	0.23766	-0.21119	# 18
C1a	-0.40225	0.01952	0.34204	# 37
C2a	-0.26471	0.04756	0.27014	# 38
C3a	-0.16685	0.01035	0.18737	# 39
C4a	-0.21119	-0.05745	0.17806	# 40
C5a	-0.34731	-0.08828	0.24752	# 41
C6a	-0.44051	-0.04852	0.32874	# 42
H16a	-0.47658	0.04946	0.40583	# 43

```
H17a     -0.06040   0.03325   0.13238                    # 44
H18a     -0.37944  -0.14113   0.23873                    # 45
N7a      -0.22073   0.11991   0.28218                   # 55
O10a     -0.30949   0.15135   0.35597                    # 56
O11a     -0.09873   0.14314   0.21749                    # 57
N8a      -0.10943  -0.09845   0.09073                   # 61
O14a     -0.15178  -0.15809   0.08467                    # 62
O15a      0.00979  -0.06978   0.03081                    # 63
N9a      -0.58625  -0.07988   0.40403                   # 67
O12a     -0.61671  -0.13998   0.39016                    # 68
O13a     -0.66590  -0.04346   0.47478                    # 69
C1a       0.07675   0.40514   0.01492                   # 73
C2a       0.04785   0.38916  -0.06002                   # 74
C3a      -0.03506   0.32986  -0.05943                    # 75
C4a      -0.08983   0.28574   0.02015                   # 76
C5a      -0.06458   0.29898   0.09722                   # 77
C6a       0.01909   0.35908   0.09258                   # 78
H16a      0.14156   0.45158   0.01289                    # 79
H17a     -0.05613   0.31850  -0.11857                    # 80
H18a     -0.10832   0.26390   0.15839                    # 81
N7a       0.10773   0.43719  -0.14377                   # 91
O10a      0.18041   0.48903  -0.14211                    # 92
O11a      0.08030   0.42163  -0.20868                    # 93
N8a      -0.17856   0.22216   0.02293                   # 97
O14a     -0.22528   0.18431   0.09411                    # 98
O15a     -0.19885   0.21196  -0.04614                    # 99
N9a       0.04793   0.37464   0.17354                   #103
O12a     -0.00445   0.33299   0.24096                    #104
O13a      0.12210   0.42804   0.16728                    #105
#END



data_ BTF-1,3,5-trinitrobenzene(1:3)_-9.56424E+01
_chemical_name_systematic
;RAS tnb-d3

E(total)=-9.56424E+01 E(coul)=-2.25486E+01 E(vdW)=-7.30938E+01 Density= 1.76039
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_cell_length_a   16.123
_cell_length_b   11.753
_cell_length_c    9.955
_cell_angle_alpha    90.00
_cell_angle_beta     63.07
_cell_angle_gamma    90.00
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P 21    '
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  2 -x,1/2+y,-z
loop_
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       0.05317   0.33650   0.43852                    #  1
C2       0.13893   0.27588   0.38936                    #  2
C3       0.15556   0.16909   0.31048                    #  3
C4       0.08279   0.12389   0.28166                    #  4
C5      -0.00482   0.18146   0.32870                    #  5
C6      -0.01780   0.28728   0.40666                    #  6
N7       0.19371   0.33605   0.43013                    #  7
O8       0.13722   0.43820   0.50792                    #  8
N'9      0.05293   0.43142   0.50780                    #  9
N'10     0.22904   0.10308   0.25809                    # 10
O11      0.20884   0.01232   0.19301                    # 11
N12      0.11278   0.02598   0.20849                    # 12
N'13    -0.07805   0.15256   0.31180                    # 13
O14     -0.14215   0.23654   0.37676                    # 14
N15     -0.10258   0.32503   0.43907                    # 15
O16      0.08160  -0.04622   0.15759                    # 16
O17      0.27132   0.32602   0.41837                    # 17
O18     -0.14900   0.40725   0.50173                    # 18
C1a      0.44075   0.21609   0.42483                    # 37
C2a      0.39909   0.11647   0.40995                    # 38
C3a      0.32136   0.06920   0.52864                    # 39
C4a      0.28536   0.12558   0.66633                    # 40
C5a      0.32400   0.22543   0.68801                    # 41
C6a      0.40167   0.26867   0.56520                    # 42
H16a     0.50120   0.25130   0.33089                    # 43
H17a     0.29012  -0.00840   0.51441                    # 44
H18a     0.29479   0.26782   0.79618                    # 45
N7a      0.43908   0.05844   0.26186                    # 55
O10a     0.50764   0.10228   0.15946                    # 56
O11a     0.40074  -0.02923   0.25239                    # 57
N8a      0.20260   0.07737   0.79494                    # 61
O14a     0.17252   0.12910   0.91486                    # 62
O15a     0.17016  -0.01077   0.77218                    # 63
N9a      0.44444   0.37490   0.58468                    # 67
O12a     0.40833   0.41922   0.70985                    # 68
O13a     0.51285   0.41085   0.47422                    # 69
C1a      0.64328   0.01992  -0.16970                    # 73
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C2a 0.61036 -0.08260 -0.09452 # 74
C3a 0.52302 -0.12566 -0.06251 # 75
C4a 0.46794 -0.06189 -0.10883 # 76
C5a 0.49708 0.04118 -0.18440 # 77
C6a 0.58509 0.07993 -0.21326 # 78
H16a 0.71149 0.05175 -0.19338 # 79
H17a 0.49887 -0.20564 -0.00387 # 80
H18a 0.45302 0.08933 -0.21936 # 81
N7a 0.67068 -0.14852 -0.04665 # 91
O10a 0.74730 -0.10824 -0.07656 # 92
O11a 0.63964 -0.23859 0.01941 # 93
N8a 0.37455 -0.10547 -0.07641 # 97
O14a 0.32767 -0.04724 -0.11873 # 98
O15a 0.35089 -0.19661 -0.00960 # 99
N9a 0.61815 0.18943 -0.29354 #103
O12a 0.56519 0.24030 -0.33045 #104
O13a 0.69608 0.22127 -0.31729 #105
C1a -0.05937 -0.01434 -0.07170 #109
C2a -0.09751 -0.06550 0.06957 #110
C3a -0.17485 -0.02167 0.19239 #111
C4a -0.21415 0.07728 0.16978 #112
C5a -0.17909 0.13223 0.03117 #113
C6a -0.10165 0.08442 -0.08749 #114
H16a 0.00085 -0.04999 -0.16564 #115
H17a -0.20333 -0.06295 0.30127 #116
H18a -0.21083 0.20914 0.01623 #117
N7a -0.05407 -0.17080 0.09002 #127
O10a 0.01404 -0.20730 -0.02048 #128
O11a -0.08935 -0.21386 0.21597 #129
N8a -0.29658 0.12608 0.29839 #133
O14a -0.32962 0.21341 0.27480 #134
O15a -0.32582 0.07562 0.41914 #135
N9a -0.06266 0.14093 -0.23655 #139
O12a -0.10153 0.22789 -0.24681 #140
O13a 0.00566 0.09666 -0.33891 #141
#END

Simulated cocrystal structures of BTF-1,2,3,3,5,6-hexanitrobenzene

data_BTF-HNB(1:1)_-5.56486E+01
_chemical_name_systematic
;RAS HNBZ

E(total)=-5.56486E+01 E(coul)=-1.11877E+01 E(vdW)=-4.44610E+01 Density= 1.99232
;

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_cell_length_a   23.580
_cell_length_b    8.859
_cell_length_c    9.582
_cell_angle_alpha    90.00
_cell_angle_beta     91.35
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.42867  -0.08899  -0.51702                    #  1
C2        0.40782  -0.19725  -0.41978                    #  2
C3        0.36474  -0.15987  -0.32130                    #  3
C4        0.34273  -0.00919  -0.32261                    #  4
C5        0.36237   0.10362  -0.41847                    #  5
C6        0.40523   0.06121  -0.51440                    #  6
N7        0.43516  -0.32627  -0.44096                    #  7
O8        0.47427  -0.29317  -0.55668                    #  8
N'9       0.46760  -0.14658  -0.59668                    #  9
N'10      0.34105  -0.24371  -0.22617                    # 10
O11       0.30288  -0.15411  -0.16108                    # 11
N12       0.30399  -0.00070  -0.22420                    # 12
N'13      0.34713   0.24506  -0.43395                    # 13
O14       0.37863   0.30205  -0.53903                    # 14
N15       0.41663   0.18175  -0.59163                    # 15
O16       0.27275   0.09582  -0.18001                    # 16
O17       0.43484  -0.45184  -0.39085                    # 17
O18       0.44819   0.21078  -0.68593                    # 18
C1A       0.11410  -0.12768  -0.06283                    # 73
C2A       0.08714   0.00550  -0.10364                    # 74
C3A       0.10967   0.14419  -0.06251                    # 75
C4A       0.15916   0.14970   0.01941                    # 76
C5A       0.18612   0.01652   0.06022                    # 77
C6A       0.16359  -0.12217   0.01909                    # 78
N7A       0.09003  -0.27580  -0.10675                    # 79
O8A       0.08135  -0.36545  -0.01299                    # 80
O9A       0.08150  -0.29211  -0.23193                    # 81
```

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N10A      0.03428  -0.00038  -0.19113                    # 82
O11A      0.03470   0.07271  -0.29902                    # 83
O12A     -0.00395  -0.07769  -0.14584                    # 84
N13A      0.08088   0.28642  -0.10609                    # 85
O14A      0.11033   0.37839  -0.16547                    # 86
O15A      0.03083   0.29621  -0.07788                    # 87
N16A      0.18323   0.29782   0.06333                    # 88
O17A      0.23277   0.31924   0.03516                    # 89
O18A      0.15090   0.38236   0.12292                    # 90
N19A      0.23898   0.02240   0.14771                    # 91
O20A      0.27958  -0.04558   0.10224                    # 92
O21A      0.23620   0.09460   0.25577                    # 93
N22A      0.19238  -0.26440   0.06267                    # 94
O23A      0.20142  -0.27931   0.18781                    # 95
O24A      0.20394  -0.35126  -0.03130                    # 96
#END
```