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Structure and complexation energy of benzotrifuroxan–benzene molecular complex

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The atoms and charges coordinate of BTF and benzene molecules:

Benzotrifuroxan molecules with coordinates of atoms, site charges (X element number) and additional site charges (XLP number), +/- above and below the plane of molecules

C1	-1.254037	0.730100	0.000000
C2	0.000000	1.421992	0.000000
C3	1.259304	0.720978	0.000000
C4	1.231481	-0.710996	0.000000
C5	-0.005267	-1.451078	0.000000
C6	-1.231481	-0.710996	0.000000
N7	-0.261911	2.726166	0.000000
O8	-1.747273	2.815568	0.000000
N'9	-2.270579	1.557976	0.000000
N'10	2.484537	1.187391	0.000000
O11	3.311990	0.105398	0.000000
N12	2.491884	-1.136262	0.000000
N'13	-0.213957	-2.745368	0.000000
O14	-1.564717	-2.920967	0.000000
N15	-2.229974	-1.589904	0.000000
O16	3.051105	-2.211188	0.000000
O17	0.389393	3.747929	0.000000
O18	-3.440498	-1.536740	0.000000

Artificial atoms for charges of Benzotrifuroxan

XC1	-1.566407	0.199933	0.000000
XC2	-0.094581	1.403229	0.000000
XC3	0.956350	1.256582	0.000000
XC4	1.262522	-0.619705	0.000000
XC5	0.610057	-1.456515	0.000000
XC6	-1.167941	-0.783524	0.000000
XN7	-0.173049	2.603666	0.000000
XO8	-1.896787	2.770290	0.000000
XN'9	-2.403895	1.532497	0.000000
XN'10	2.529129	1.315585	0.000000
XO11	3.347535	0.257521	0.000000
XN12	2.341365	-1.151968	0.000000
XN'13	-0.125234	-2.848083	0.000000
XO14	-1.450748	-3.027811	0.000000
XN15	-2.168316	-1.451698	0.000000
XO16	2.842284	-1.683654	0.000000
XO17	0.036945	3.303317	0.000000
XO18	-2.879229	-1.619663	0.000000

Artificial atoms for charges of Benzotrifuroxan

XLP1+	-1.106216	0.769186	0.258692
XLP1-	-1.106216	0.769186	-0.258692
XLP2+	-0.214908	1.791996	0.648878
XLP2-	-0.214908	1.791996	-0.648878
XLP3+	1.219243	0.573418	0.258692
XLP3-	1.219243	0.573418	-0.258692
XLP4+	1.659368	-0.709882	0.648878
XLP4-	1.659368	-0.709882	-0.648878
XLP5+	-0.113027	-1.342604	0.258692
XLP5-	-0.113027	-1.342604	-0.258692
XLP6+	-1.444460	-1.082114	0.648878
XLP6-	-1.444460	-1.082114	-0.648878
XLP7+	-0.357166	2.687572	0.033695
XLP7-	-0.357166	2.687572	-0.033695
XLP8+	-2.351721	2.731502	-0.020272
XLP8-	-2.351721	2.731502	0.020272
XLP9+	-2.961694	1.354973	0.405377
XLP9-	-2.961694	1.354973	-0.405377
XLP10+	2.654289	1.887416	0.405377
XLP10-	2.654289	1.887416	-0.405377
XLP11+	3.541410	0.670899	-0.020272
XLP11-	3.541410	0.670899	0.020272
XLP12+	2.506089	-1.034472	0.033695
XLP12-	2.506089	-1.034472	-0.033695
XLP13+	0.307406	-3.242389	0.405377
XLP13-	0.307406	-3.242389	-0.405377
XLP14+	-1.189690	-3.402401	-0.020272
XLP14-	-1.189690	-3.402401	0.020272
XLP15+	-2.148923	-1.653101	0.033695
XLP15-	-2.148923	-1.653101	-0.033695
XLP16+	2.916498	-1.882922	0.304294
XLP16-	2.916498	-1.882922	-0.304294
XLP17+	0.172409	3.467222	0.304294
XLP17-	0.172409	3.467222	-0.304294
XLP18+	-3.088907	-1.584300	0.304294
XLP18-	-3.088907	-1.584300	-0.304294

Benzene molecule with coordinates of atoms, site charges (X - element number ‘A’) and additional site charges (XA number), +/- above and below the plane of molecules

C1A	0.000000	1.397607	0.000000
C2A	1.210363	0.698803	0.000000
C3A	1.210363	-0.698803	0.000000
C4A	0.000000	-1.397607	0.000000
C5A	-1.210363	-0.698803	0.000000
C6A	-1.210363	0.698803	0.000000
H7A	0.000000	2.484537	0.000000
H8A	2.151672	1.242268	0.000000
H9A	2.151672	-1.242268	0.000000
H10A	0.000000	-2.484537	0.000000

H11A	-2.151672	-1.242268	0.000000
H12A	-2.151672	1.242268	0.000000

Artificial atoms for charges

XC1A	-0.000343	1.326381	-0.000085
XC2A	1.148508	0.663488	-0.000085
XC3A	1.148852	-0.662893	-0.000085
XC4A	0.000343	-1.326381	-0.000085
XC5A	-1.148508	-0.663488	-0.000085
XC6A	-1.148852	0.662893	-0.000085
XH7A	-0.000003	2.323275	-0.000027
XH8A	2.012014	1.161641	-0.000027
XH9A	2.012017	-1.161635	-0.000027
XH10A	0.000003	-2.323275	-0.000027
XH11A	-2.012014	-1.161641	-0.000027
XH12A	-2.012017	1.161635	-0.000027

Artificial atoms for charges (A)

XA1+	-0.000002	-0.144548	-0.264499
XA1-	0.000002	-0.144548	0.264499
XA2+	-0.125183	-0.072273	-0.264499
XA2-	-0.125182	-0.072276	0.264499
XA3+	-0.125182	0.072276	-0.264499
XA3-	-0.125183	0.072273	0.264499
XA4+	0.000002	0.144548	-0.264499
XA4-	-0.000002	0.144548	0.264499
XA5+	0.125183	0.072273	-0.264499
XA5-	0.125182	0.072276	0.264499
XA6+	0.125182	-0.072276	-0.264499
XA6-	0.125183	-0.072273	0.264499
XA7+	0.000007	2.280204	0.238965
XA7-	-0.000007	2.280204	-0.238965
XA8+	1.974718	1.140096	0.238965
XA8-	1.974711	1.140108	-0.238965
XA9+	1.974711	-1.140108	0.238965
XA9-	1.974718	-1.140096	-0.238965
XA10+	-0.000007	-2.280204	0.238965
XA10-	0.000007	-2.280204	-0.238965
XA11+	-1.974718	-1.140096	0.238965
XA11-	-1.974711	-1.140108	-0.238965
XA12+	-1.974711	1.140108	0.238965
XA12-	-1.974718	1.140096	-0.238965

The charges corresponding to each site charge of BTF.

Charge C1	0.0
Charge C2	0.0
Charge C3	0.0
Charge C4	0.0
Charge C5	0.0
Charge C6	0.0
Charge N7	0.0
Charge O8	0.0

Charge N'9 0.0
Charge N'10 0.0
Charge O11 0.0
Charge N12 0.0
Charge N'13 0.0
Charge O14 0.0
Charge N15 0.0
Charge O16 0.0
Charge O17 0.0
Charge O18 0.0
Charge XC1 -0.090030
Charge XC2 0.281440
Charge XC3 -0.090030
Charge XC4 0.281440
Charge XC5 -0.090030
Charge XC6 0.281440
Charge XN7 0.529104
Charge XO8 -0.500608
Charge XN'9 0.223106
Charge XN'10 0.223106
Charge XO11 -0.500608
Charge XN12 0.529104
Charge XN'13 0.223106
Charge XO14 -0.500608
Charge XN15 0.529104
Charge XO16 -0.062445
Charge XO17 -0.062445
Charge XO18 -0.062445
Charge XLP1+ 0.014330
Charge XLP1- 0.014330
Charge XLP2+ -0.244399
Charge XLP2- -0.244399
Charge XLP3+ 0.014330
Charge XLP3- 0.014330
Charge XLP4+ -0.244399
Charge XLP4- -0.244399
Charge XLP5+ 0.014330
Charge XLP5- 0.014330
Charge XLP6+ -0.244399
Charge XLP6- -0.244399
Charge XLP7+ 0.361716
Charge XLP7- 0.361716
Charge XLP8+ 0.104390
Charge XLP8- 0.104390
Charge XLP9+ -0.132572
Charge XLP9- -0.132572
Charge XLP10+ -0.132572
Charge XLP10- -0.132572
Charge XLP11+ 0.104390
Charge XLP11- 0.104390
Charge XLP12+ 0.361716
Charge XLP12- 0.361716

Charge XLP13+ -0.132572
Charge XLP13- -0.132572
Charge XLP14+ 0.104390
Charge XLP14- 0.104390
Charge XLP15+ 0.361716
Charge XLP15- 0.361716
Charge XLP16+ -0.293748
Charge XLP16- -0.293748
Charge XLP17+ -0.293748
Charge XLP17- -0.293748
Charge XLP18+ -0.293748
Charge XLP18- -0.293748

The charges corresponding to the each site charge of Benzene.
Charge C1A 0.0
Charge C2A 0.0
Charge C3A 0.0
Charge C4A 0.0
Charge C5A 0.0
Charge C6A 0.0
Charge H7A 0.0
Charge H8A 0.0
Charge H9A 0.0
Charge H10A 0.0
Charge H11A 0.0
Charge H12A 0.0
Charge XC1A -0.160231
Charge XC2A -0.160231
Charge XC3A -0.160231
Charge XC4A -0.160231
Charge XC5A -0.160231
Charge XC6A -0.160231
Charge XH7A 0.520343
Charge XH8A 0.520343
Charge XH9A 0.520343
Charge XH10A 0.520343
Charge XH11A 0.520343
Charge XH12A 0.520343
Charge XA1+ 0.019554
Charge XA1- 0.019554
Charge XA2+ 0.019554
Charge XA2- 0.019554
Charge XA3+ 0.019554
Charge XA3- 0.019554
Charge XA4+ 0.019554
Charge XA4- 0.019554
Charge XA5+ 0.019554
Charge XA5- 0.019554
Charge XA6+ 0.019554
Charge XA6- 0.019554
Charge XA7+ -0.199609
Charge XA7- -0.199609

Charge XA8+ -0.199609
Charge XA8- -0.199609
Charge XA9+ -0.199609
Charge XA9- -0.199609
Charge XA10+ -0.199609
Charge XA10- -0.199609
Charge XA11+ -0.199609
Charge XA11- -0.199609
Charge XA12+ -0.199609
Charge XA12- -0.199609

Additional information on the content of crystal packing models of BTF-benzene complex in cif format:

Model C1

data_____-4.17327E+01
_chemical_name_systematic
;RAS BTFO_C3H

E(total) = -4.17327E+01 E(coul) = -1.07868E+01 E(vdW) = -3.09459E+01 Density= 1.69;
_cell_length_a 7.135
_cell_length_b 11.901
_cell_length_c 16.655
_cell_angle_alpha 90.00
_cell_angle_beta 113.53
_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	-0.66425	0.85099	0.42397	# 1
C2	-0.73953	0.82264	0.33293	# 2
C3	-0.68627	0.71865	0.30292	# 3
C4	-0.55383	0.64264	0.36727	# 4
C5	-0.47426	0.66748	0.45960	# 5
C6	-0.53142	0.77185	0.48629	# 6
N'7	-0.85754	0.90693	0.28820	# 7
O8	-0.85228	0.98969	0.35605	# 8
N'9	-0.73143	0.94911	0.43667	# 9
N'10	-0.74047	0.67961	0.22319	# 10
O11	-0.64812	0.57767	0.23081	# 11

```
N'12     -0.52604   0.55352   0.32508                    # 12
N'13     -0.35288   0.60841   0.52664                    # 13
O14      -0.32438   0.66977   0.59964                    # 14
N'15     -0.44120   0.77668   0.57322                    # 15
O16      -0.43189   0.46603   0.34535                    # 16
O17      -0.95779   0.92805   0.21177                    # 17
O18      -0.43510   0.84305   0.62938                    # 18
#XC1     -0.61019   0.83880   0.46457                    # 19
#XC2     -0.74050   0.82910   0.33695                    # 20
#XC3     -0.73591   0.76564   0.29289                    # 21
#XC4     -0.56165   0.64325   0.36052                    # 22
#XC5     -0.47868   0.63269   0.42904                    # 23
#XC6     -0.52263   0.76478   0.48903                    # 24
#XN'7    -0.84366   0.89246   0.28999                    # 25
#XO8     -0.84282   0.99614   0.36968                    # 26
#XN'9    -0.73412   0.95635   0.43970                    # 27
#XN'10   -0.74728   0.67882   0.21632                    # 28
#XO11    -0.66879   0.58790   0.21952                    # 29
#XN'12   -0.52293   0.56294   0.33512                    # 30
#XN'13   -0.34339   0.60196   0.53048                    # 31
#XO14    -0.31317   0.65310   0.59729                    # 32
#XN'15   -0.45819   0.78174   0.56140                    # 33
#XO16    -0.47450   0.50210   0.33349                    # 34
#XO17    -0.91735   0.92284   0.24513                    # 35
#XO18    -0.43293   0.81219   0.60788                    # 36
#XLP1+   -0.69943   0.83711   0.41425                    # 37
#XLP1-   -0.64345   0.85423   0.41233                    # 38
#XLP2+   -0.85484   0.82602   0.32860                    # 39
#XLP2-   -0.68760   0.87719   0.32288                    # 40
#XLP3+   -0.69796   0.70222   0.31293                    # 41
#XLP3-   -0.64199   0.71935   0.31101                    # 42
#XLP4+   -0.63883   0.59461   0.35177                    # 43
#XLP4-   -0.47159   0.64578   0.34604                    # 44
#XLP5+   -0.51135   0.67211   0.46219                    # 45
#XLP5-   -0.45538   0.68924   0.46028                    # 46
#XLP6+   -0.58197   0.73975   0.51471                    # 47
#XLP6-   -0.41473   0.79092   0.50899                    # 48
#XLP7+   -0.84962   0.91106   0.29291                    # 49
#XLP7-   -0.85928   0.90811   0.29324                    # 50
#XLP8+   -0.83300   1.01466   0.39441                    # 51
#XLP8-   -0.83037   1.01547   0.39432                    # 52
#XLP9+   -0.75171   0.95828   0.47372                    # 53
#XLP9-   -0.66971   0.98337   0.47092                    # 54
#XL10+   -0.83736   0.69124   0.19142                    # 55
#XL10-   -0.75537   0.71632   0.18861                    # 56
#XL11+   -0.71028   0.60218   0.19367                    # 57
#XL11-   -0.70765   0.60298   0.19358                    # 58
#XL12+   -0.52873   0.55847   0.32062                    # 59
#XL12-   -0.53838   0.55551   0.32095                    # 60
#XL13+   -0.35870   0.54998   0.52557                    # 61
#XL13-   -0.27671   0.57507   0.52276                    # 62
#XL14+   -0.28544   0.61908   0.59855                    # 63
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#XL14-     -0.28281   0.61989   0.59846                  # 64
#XL15+     -0.43195   0.77203   0.57248                  # 65
#XL15-     -0.44160   0.76908   0.57281                  # 66
#XL16+     -0.49679   0.47944   0.33915                  # 67
#XL16-     -0.42372   0.50180   0.33665                  # 68
#XL17+     -0.96659   0.91269   0.23543                  # 69
#XL17-     -0.89353   0.93505   0.23293                  # 70
#XL18+     -0.47100   0.81146   0.61567                  # 71
#XL18-     -0.39793   0.83382   0.61317                  # 72
C1+        0.21119   0.20311   0.66353                  # 73
C2+        0.17774   0.14096   0.58762                  # 74
C3+        0.05606   0.18536   0.50531                  # 75
C4+       -0.03217   0.29189   0.49893                  # 76
C5+        0.00128   0.35404   0.57484                  # 77
C6+        0.12296   0.30964   0.65715                  # 78
H7+        0.30596   0.16853   0.72763                  # 79
H8+        0.24646   0.05799   0.59259                  # 80
H9+        0.03001   0.13696   0.44619                  # 81
H10+      -0.12694   0.32647   0.43483                  # 82
H11+      -0.06744   0.43701   0.56987                  # 83
H12+       0.14901   0.35804   0.71627                  # 84
#XC1+      0.25170   0.19080   0.69271                  # 85
#XC2+      0.21036   0.10499   0.59242                  # 86
#XC3+      0.04816   0.16169   0.48095                  # 87
#XC4+     -0.07268   0.30420   0.46975                  # 88
#XC5+     -0.03134   0.39001   0.57004                  # 89
#XC6+      0.13086   0.33331   0.68151                  # 90
#XH7+      0.36349   0.14577   0.76528                  # 91
#XH8+      0.28585   0.00798   0.59369                  # 92
#XH9+      0.01187   0.10971   0.40964                  # 93
#XH10+    -0.18447   0.34923   0.39718                  # 94
#XH11+    -0.10683   0.48702   0.56877                  # 95
#XH12+     0.16715   0.38529   0.75282                  # 96
#XP1+      0.31987   0.22195   0.68193                  # 97
#XP1-      0.15762   0.16416   0.68241                  # 98
#XP2+      0.28566   0.14083   0.59171                  # 99
#XP2-      0.10977   0.09285   0.58642                  #100
#XP3+      0.13821   0.18979   0.48851                  #101
#XP3-     -0.04124   0.15278   0.48774                  #102
#XP4+      0.02496   0.31988   0.47553                  #103
#XP4-     -0.14441   0.28401   0.48505                  #104
#XP5+      0.05916   0.40100   0.56576                  #105
#XP5-     -0.09656   0.35532   0.58104                  #106
#XP6+      0.20662   0.35203   0.66896                  #107
#XP6-      0.05445   0.29540   0.67972                  #108
#END
```

Model C2

```
data_____-4.15314E+01
_chemical_name_systematic
;RAS BTFO_C3H
```

```
E(total)= - 4.15314E+01     E(coul = - 1.14956E+01   E(vdW) = -3.00357E+01      Density= 1.71
        ;
        _cell_length_a   15.081
        _cell_length_b    6.884
        _cell_length_c   14.194
        _cell_angle_alpha    90.00
        _cell_angle_beta    119.18
        _cell_angle_gamma    90.00
        _cell_formula_units_Z  4
        _symmetry_space_group_name_H-M 'P 21/N  '
        _symmetry_Int_Tables_number  14
        loop_
        _symmetry_equiv_pos_as_xyz
          1 x,y,z
          2 1/2-x,1/2+y,1/2-z
          3 -x,-y,-z
          4 1/2+x,1/2-y,1/2+z
        loop_
        _atom_site_label
        _atom_site_fract_x
        _atom_site_fract_y
        _atom_site_fract_z
        C1        0.01373   0.09124   0.64573                          #  1
        C2        0.09710   0.03304   0.74727                          #  2
        C3        0.08205  -0.04766   0.83212                          #  3
        C4       -0.02004  -0.06894   0.81250                          #  4
        C5       -0.10635  -0.01246   0.71166                          #  5
        C6       -0.08763   0.06703   0.62974                          #  6
        N'7       0.18220   0.06828   0.74382                          #  7
        O8        0.14776   0.15171   0.63470                          #  8
        N'9       0.04441   0.16055   0.58045                          #  9
        N'10      0.14868  -0.10786   0.92876                          # 10
        O11       0.09482  -0.17079   0.97690                          # 11
        N'12     -0.01555  -0.14530   0.90082                          # 12
        N'13     -0.20366  -0.02157   0.68031                          # 13
        O14      -0.25315   0.05021   0.57792                          # 14
        N'15     -0.17722   0.10814   0.54487                          # 15
        O16      -0.07627  -0.19330   0.92914                          # 16
        O17       0.27237   0.04861   0.80468                          # 17
        O18      -0.20668   0.17582   0.45570                          # 18
        #XC1     -0.03461   0.10105   0.61394                           # 19
        #XC2      0.09576   0.03899   0.73996                           # 20
        #XC3      0.11376  -0.02150   0.81610                           # 21
        #XC4     -0.01264  -0.07150   0.81856                           # 22
        #XC5     -0.08972  -0.04843   0.75947                           # 23
        #XC6     -0.09369   0.06363   0.63099                           # 24
        #XN'7     0.17381   0.05965   0.74999                           # 25
        #XO8      0.13627   0.16185   0.61830                           # 26
        #XN'9     0.04447   0.16659   0.57365                           # 27
        #XN'10    0.15558  -0.11138   0.93569                           # 28
        #XO11     0.11133  -0.16907   0.98203                           # 29
```

#XN'12	-0.02191	-0.13480	0.88621	# 30
#XN'13	-0.21062	-0.02408	0.68017	# 31
#XO14	-0.25817	0.03835	0.58919	# 32
#XN'15	-0.16247	0.10627	0.55331	# 33
#XO16	-0.04753	-0.17504	0.92078	# 34
#XO17	0.23482	0.05980	0.77594	# 35
#XO18	-0.19786	0.14637	0.49280	# 36
#XLP1+	0.02195	0.05238	0.65199	# 37
#XLP1-	0.02328	0.11385	0.66546	# 38
#XLP2+	0.11571	-0.04310	0.71822	# 39
#XLP2-	0.11970	0.14055	0.75846	# 40
#XLP3+	0.06829	-0.07955	0.82110	# 41
#XLP3-	0.06963	-0.01808	0.83457	# 42
#XLP4+	-0.01274	-0.18339	0.82195	# 43
#XLP4-	-0.00874	0.00027	0.86220	# 44
#XLP5+	-0.10282	-0.03391	0.69622	# 45
#XLP5-	-0.10148	0.02756	0.70969	# 46
#XLP6+	-0.11953	-0.01787	0.58897	# 47
#XLP6-	-0.11554	0.16579	0.62922	# 48
#XLP7+	0.17836	0.07743	0.73893	# 49
#XLP7-	0.17813	0.06683	0.73661	# 50
#XLP8+	0.11868	0.18350	0.58435	# 51
#XLP8-	0.11875	0.18638	0.58498	# 52
#XLP9+	0.01556	0.14523	0.52506	# 53
#XLP9-	0.01752	0.23527	0.54479	# 54
#XL10+	0.19358	-0.15167	0.93716	# 55
#XL10-	0.19554	-0.06163	0.95689	# 56
#XL11+	0.14524	-0.17229	0.99824	# 57
#XL11-	0.14530	-0.16940	0.99887	# 58
#XL12+	-0.00934	-0.13962	0.90416	# 59
#XL12-	-0.00957	-0.15022	0.90184	# 60
#XL13+	-0.22265	-0.09749	0.69770	# 61
#XL13-	-0.22069	-0.00745	0.71743	# 62
#XL14+	-0.27458	0.01559	0.60598	# 63
#XL14-	-0.27452	0.01847	0.60661	# 64
#XL15+	-0.17925	0.10922	0.54990	# 65
#XL15-	-0.17948	0.09861	0.54758	# 66
#XL16+	-0.05822	-0.22070	0.91405	# 67
#XL16-	-0.05647	-0.14046	0.93164	# 68
#XL17+	0.24597	0.01557	0.77695	# 69
#XL17-	0.24771	0.09580	0.79453	# 70
#XL18+	-0.20094	0.11590	0.47214	# 71
#XL18-	-0.19919	0.19614	0.48972	# 72
C1+	0.15415	0.50779	0.32160	# 73
C2+	0.11079	0.43968	0.38297	# 74
C3+	0.00499	0.43285	0.33783	# 75
C4+	-0.05746	0.49412	0.23133	# 76
C5+	-0.01410	0.56222	0.16997	# 77
C6+	0.09171	0.56906	0.21510	# 78
H7+	0.23655	0.51311	0.35675	# 79
H8+	0.15942	0.39197	0.46591	# 80
H9+	-0.02878	0.37981	0.38563	# 81

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H10+     -0.13986   0.48880   0.19618                    # 82
H11+     -0.06273   0.60994   0.08702                    # 83
H12+      0.12548   0.62210   0.16730                    # 84
#XC1+      0.18985   0.51227   0.33417                    # 85
#XC2+      0.13453   0.42007   0.41895                    # 86
#XC3+     -0.00698   0.40876   0.36125                    # 87
#XC4+     -0.09316   0.48964   0.21876                    # 88
#XC5+     -0.03784   0.58184   0.13398                    # 89
#XC6+      0.10367   0.59315   0.19169                    # 90
#XH7+      0.28624   0.51476   0.37985                    # 91
#XH8+      0.18683   0.36243   0.51589                    # 92
#XH9+     -0.05106   0.34862   0.41251                    # 93
#XH10+    -0.18955   0.48714   0.17308                    # 94
#XH11+    -0.09014   0.63948   0.03704                    # 95
#XH12+     0.14775   0.65329   0.14042                    # 96
#XP1+      0.17724   0.42306   0.30883                    # 97
#XP1-      0.17898   0.59561   0.35481                    # 98
#XP2+      0.12952   0.33776   0.38903                    # 99
#XP2-      0.12033   0.51386   0.42514                    #100
#XP3+      0.00038   0.32518   0.33913                    #101
#XP3-     -0.01005   0.50968   0.36433                    #102
#XP4+     -0.08105   0.39789   0.20904                    #103
#XP4-     -0.08178   0.58726   0.23319                    #104
#XP5+     -0.03334   0.48318   0.12885                    #105
#XP5-     -0.02314   0.66901   0.16285                    #106
#XP6+      0.09580   0.49577   0.17875                    #107
#XP6-      0.10724   0.67319   0.22366                    #108
#END
```

Figure S1 shows the general view of the unit cell (u.c.) for the **C-1** model in different projections.

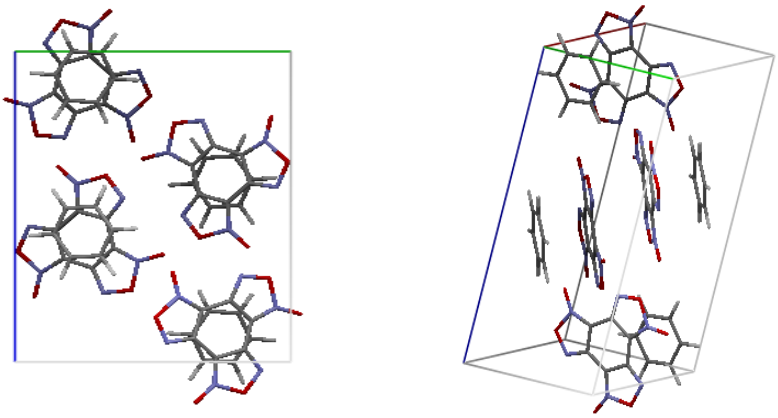

Figure S1. Packing model **C-1** of the BTF–benzene cocrystal with the lowest energy.

In Figure S2 the distance **d** (abscissa) is taken as the zero point. An increase in distance between pairs by 0.1 Å corresponds to the point 0.1, and a decrease by 0.1 Å - to the point –0.1, respectively.

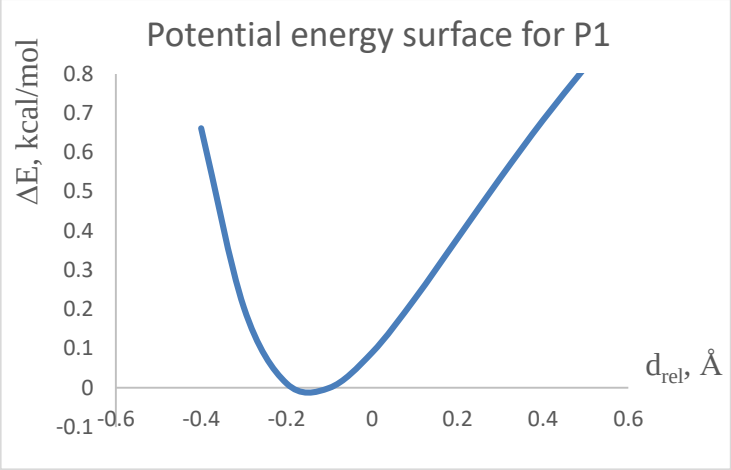

Figure S2. A characteristic curve of the potential energy of the BTF-benzene pair **P1** (see Figure 3 in the main text) in the coordinates "the relative distance between the geometric centers of molecules $\mathbf{d_{rel}}$ (Å) – potential energy ΔE (kcal·mol^{-1}).

The graph shows that at the distance between the centers of molecules **d** = 7.564 Å, taken from the **P1** model (Table 3 in the main text), the curve has not yet reached its minimum value (point 0 on the ordinate), and the minimum potential energy is at the mark d_{opt} = 7.564 – 0.1 = 7.464 Å (point –0.1 on the ordinate).