Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

A quantitative measure of halogen bond activation in cocrystallization

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Table S1. Atomic coordinates of all the molecular models employed in this work.
For each atom: x,y,z (angstrom), atomic species indicator (codes: 41 fluorine, 44 iodine, 11 acetylenic carbon, 12 aromatic carbon, 20 nitro nitrogen, 30 nitro oxygen, 18 pyrazine nitrogen, 2 hydrogen.
See also Table 1 of the CLP manual available at www.angelogavezzotti.it for all parameters used in the PIXEL calculations.

```
pyrazine
 10
  1   0.0   0.00000   0.00000 18
  2   0.0   1.12790   0.70480 12
  3   0.0   1.12790   2.09480 12
  4   0.0   0.00000   2.79960 18
  5   0.0  -1.12790   2.09480 12
  6   0.0  -1.12790   0.70480 12
  7   0.0   2.07249   0.18121  2
  8   0.0   2.07249   2.61839  2
  9   0.0  -2.07249   2.61839  2
 10   0.0  -2.07249   0.18121  2

pentafluoroiodobenzene
 12
  1   0.0   0.00000   0.00000 44
  2   0.0   0.00000  -2.08000 12
  3   0.0   1.19510  -2.77000 12
  4   0.0   1.19510  -4.15000 12
  5   0.0   0.00000  -4.84000 12
  6   0.0  -1.19510  -4.15000 12
  7   0.0  -1.19510  -2.77000 12
  8   0.0   2.35560  -2.10000 41
  9   0.0   2.35560  -4.82000 41
 10   0.0   0.00000  -6.22000 41
 11   0.0  -2.35560  -4.82000 41
 12   0.0  -2.35560  -2.10000 41
```

```
iodo-3,5-dinitrobenzene
 16
  1   0.0   0.00000   0.00000 44
  2   0.0   0.00000  -2.10000 12
  3   0.0   1.19940  -2.79250 12
  4   0.0   1.19940  -4.17750 12
  5   0.0   0.00000  -4.87000 12
  6   0.0  -1.19940  -4.17750 12
  7   0.0  -1.19940  -2.79250 12
  8   0.0   2.47246  -4.91249 20
  9   0.0   3.50708  -4.26598 30
 10   0.0   2.42990  -6.13175 30
 11   0.0  -2.47246  -4.91249 20
 12   0.0  -2.42990  -6.13175 30
 13   0.0  -3.50708  -4.26598 30
 14   0.0   2.13480  -2.25250  2
 15   0.0   0.00000  -5.95000  2
 16   0.0  -2.13480  -2.25250  2



 iodobenzene
 12
  1   0.0   0.00000   0.00000 44
  2   0.0   0.00000  -2.10000 12
  3   0.0   1.19940  -2.79250 12
  4   0.0   1.19940  -4.17750 12
  5   0.0   0.00000  -4.87000 12
  6   0.0  -1.19940  -4.17750 12
  7   0.0  -1.19940  -2.79250 12
  8   0.0   2.13480  -2.25250  2
  9   0.0   2.13480  -4.71750  2
 10   0.0   0.00000  -5.95000  2
 11   0.0  -2.13480  -4.71750  2
 12   0.0  -2.13480  -2.25250  2

iodo-4-nitrobenzene
 14
  1   0.0   0.00000   0.00000 44
  2   0.0   0.00000  -2.10000 12
  3   0.0   1.19940  -2.79250 12
  4   0.0   1.19940  -4.17750 12
  5   0.0   0.00000  -4.87000 12
  6   0.0  -1.19940  -4.17750 12
  7   0.0  -1.19940  -2.79250 12
  8   0.0   0.00000  -6.34000 20
  9   0.0   1.07720  -6.91275 30
 10   0.0  -1.07720  -6.91275 30
 11   0.0   2.13480  -2.25250  2
 12   0.0   2.13480  -4.71750  2
 13   0.0  -2.13480  -4.71750  2
 14   0.0  -2.13480  -2.25250  2

iodoethynylbenzene
 14
  1   0.0   0.00000   0.00000 44
  2   0.0   0.00000  -2.01000 11
```

```
  3   0.0   0.00000  -3.21000 11
  4   0.0   0.00000  -4.65000 12
  5   0.0   1.19940  -5.34250 12
  6   0.0   1.19940  -6.72750 12
  7   0.0   0.00000  -7.42000 12
  8   0.0  -1.19940  -6.72750 12
  9   0.0  -1.19940  -5.34250 12
 10   0.0   2.13480  -4.80250  2
 11   0.0   2.13480  -7.26750  2
 12   0.0   0.00000  -8.50000  2
 13   0.0  -2.13480  -7.26750  2
 14   0.0  -2.13480  -4.80250  2
```

```
iodoethynyl-4-nitrobenzene
 16
  1   0.0   0.00000   0.00000 44
  2   0.0   0.00000  -2.01000 11
  3   0.0   0.00000  -3.21000 11
  4   0.0   0.00000  -4.65000 12
  5   0.0   1.19940  -5.34250 12
  6   0.0   1.19940  -6.72750 12
  7   0.0   0.00000  -7.42000 12
  8   0.0  -1.19940  -6.72750 12
  9   0.0  -1.19940  -5.34250 12
 10   0.0   0.00000  -8.89000 20
 11   0.0   1.07720  -9.46275 30
 12   0.0  -1.07720  -9.46275 30
 13   0.0   2.13480  -4.80250  2
 14   0.0   2.13480  -7.26750  2
 15   0.0  -2.13480  -7.26750  2
 16   0.0  -2.13480  -4.80250  2

bromoethynil-4-nitrobenzene
 16
  1   0.0   0.00000   0.00000 43
  2   0.0   0.00000  -1.80000 11
  3   0.0   0.00000  -3.00000 11
  4   0.0   0.00000  -4.44000 12
  5   0.0   1.19940  -5.13250 12
  6   0.0   1.19940  -6.51750 12
  7   0.0   0.00000  -7.21000 12
  8   0.0  -1.19940  -6.51750 12
  9   0.0  -1.19940  -5.13250 12
 10   0.0   0.00000  -8.68000 20
 11   0.0   1.07720  -9.25275 30
 12   0.0  -1.07720  -9.25275 30
 13   0.0   2.13480  -4.59250  2
 14   0.0   2.13480  -7.05750  2
```

```
 15   0.0  -2.13480  -7.05750  2
 16   0.0  -2.13480  -4.59250  2

chloroethynyl-4-nitrobenzene
 16
  1   0.0   0.00000   0.00000 42
  2   0.0   0.00000  -1.63000 11
  3   0.0   0.00000  -2.83000 11
  4   0.0   0.00000  -4.27000 12
  5   0.0   1.19940  -4.96250 12
  6   0.0   1.19940  -6.34750 12
  7   0.0   0.00000  -7.04000 12
  8   0.0  -1.19940  -6.34750 12
  9   0.0  -1.19940  -4.96250 12
 10   0.0   0.00000  -8.51000 20
 11   0.0   1.07720  -9.08275 30
 12   0.0  -1.07720  -9.08275 30
 13   0.0   2.13480  -4.42250  2
 14   0.0   2.13480  -6.88750  2
 15   0.0  -2.13480  -6.88750  2
 16   0.0  -2.13480  -4.42250  2



iodoethynyl-3,5-dinitrobenzene
 18
  1   0.0   0.00000   0.00000 44
  2   0.0   0.00000  -2.01000 11
  3   0.0   0.00000  -3.21000 11
  4   0.0   0.00000  -4.65000 12
  5   0.0   1.19940  -5.34250 12
  6   0.0   1.19940  -6.72750 12
  7   0.0   0.00000  -7.42000 12
  8   0.0  -1.19940  -6.72750 12
  9   0.0  -1.19940  -5.34250 12
 10   0.0   2.47246  -7.46249 20
 11   0.0   3.50708  -6.81598 30
 12   0.0   2.42990  -8.68175 30
 13   0.0  -2.47246  -7.46249 20
 14   0.0  -3.50708  -6.81598 30
 15   0.0  -2.42990  -8.68175 30
 16   0.0   2.13480  -4.80250  2
 17   0.0   0.00000  -8.50000  2
 18   0.0  -2.13480  -4.80250  2

 iodomethane
  5
  1   0.0       0.00000   0.00000   44
  2   0.0       0.00000  -2.16000   13
  3   0.0       1.01824  -2.52000    3
  4   0.88182  -0.50912  -2.52000    3
  5  -0.88182  -0.50912  -2.52000    3
```

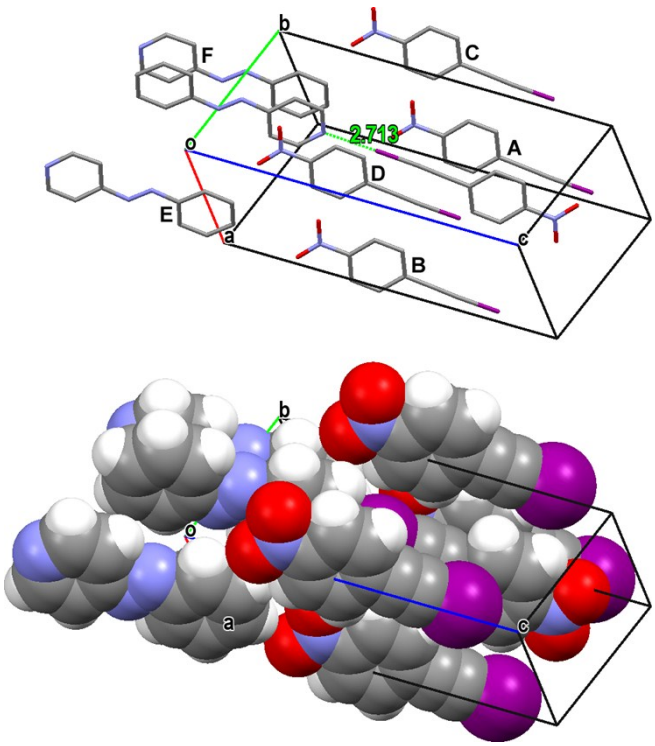

Figure S1 Stick (top) and CPK (bottom) views of the unit cell of KUXBIQ showing the six A-F interaction types involving the 1-(iodoethynyl)-4-nitrobenzene 4-(phenyldiazenyl)pyridine halogen bonded dimer (N…I = 2.713 Å). For clarity hydrogen atoms are not showed in the top view.