Supporting information

Experimental Electron Density Study of the Supramolecular Aggregation between 4,4'-dipyridyl-N,N'-dioxide and 1,4-diiodotetrafluorobenzene at 90 K

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Table S1. Atomic fractional coordinates and thermal parameters ($Å^2$ x 10^2) from the POP+CUM refinement.

T(aniso) = $\exp[-2\pi^2(U_{11}h^2a^{*2} + ... + 2U_{23}klb^*c^*)]$, T(iso) = $\exp[-2U(2\pi\sin\theta/\lambda)^2]$, where U_{ij} and U are the mean-square amplitudes of vibration.

Atom	X	Y	Z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I	0.61751(7)	0.30261(5)	0.19332(2)	1.292(10)	1.735(11)	1.443(10)	0.143(8)	0.086(8)	–0.107(9)
F1	0.33602(221)	0.29607(100)	–0.04368(54)	3.70 (8)	2.27 (5)	2.07 (5)	–0.93 (5)	0.04 (5)	0.79 (4)
F2	–0.13830(204)	0.06720(98)	–0.18793(42)	3.40 (6)	2.49 (5)	1.36 (3)	–0.16 (5)	–0.29 (4)	0.68 (3)
O	1.03431(27)	0.51013(15)	0.36844(8)	1.66 (3)	1.75 (3)	1.62 (3)	–0.52 (3)	–0.08 (2)	0.23 (3)
N	1.29651(20)	0.64053(11)	0.40300(7)	1.23 (2)	1.23 (2)	1.27 (2)	–0.03 (2)	0.05 (2)	0.21 (2)
C1	1.43108(24)	0.73095(13)	0.33832(7)	1.45 (3)	1.58 (3)	1.17 (3)	–0.13 (2)	–0.05 (2)	0.28 (2)
C2	1.70496(24)	0.87171(13)	0.37509(7)	1.47 (3)	1.52 (3)	1.20 (3)	–0.09 (2)	0.09 (2)	0.32 (2)
C3	1.85517(20)	0.92422(11)	0.47969(7)	1.10 (2)	1.18 (2)	1.23 (2)	0.06 (2)	0.11 (2)	0.23 (2)
C4	1.71144(22)	0.82543(12)	0.54328(7)	1.32 (3)	1.31 (3)	1.19 (3)	–0.09 (2)	0.03 (2)	0.25 (2)
C5	1.43440(23)	0.68731(12)	0.50483(7)	1.35 (3)	1.36 (3)	1.27 (3)	–0.06 (2)	0.15 (2)	0.32 (2)
C6	0.25673(24)	0.12134(13)	0.07682(7)	1.48 (3)	1.54 (3)	1.16 (3)	0.16 (2)	0.12 (2)	0.14 (2)
C7	0.17689(28)	0.15072(15)	–0.02026(8)	1.98 (4)	1.65 (3)	1.23 (3)	–0.13 (3)	0.07 (2)	0.31 (2)
C8	–0.07471(28)	0.03179(14)	–0.09519(7)	1.91 (3)	1.67 (3)	1.10 (3)	0.07 (3)	0.04 (2)	0.29 (2)
Atom	**X**	**Y**	**Z**	**U**					
H1	1.300(9)	0.678(5)	0.256(3)	2.0(9)					
H2	1.795(7)	0.936(4)	0.322(2)	3.4(9)					
H4	1.782(7)	0.849(4)	0.626(3)	4.1(10)					
H5	1.305(8)	0.613(4)	0.550(2)	3.1(10)					

Table S2. Third order Gram-Charlier coefficients Cijk scaled by 10^4 for the iodine and fluorine atoms from the POP+CUM refinement.

Cijk	I	F1	F2
C111	–0.09(9)	–12.4(30)	–4.9(25)
C112	0.17(7)	6.5(17)	3.8(15)
C122	–0.08(4)	–1.5(8)	0.1(8)
C113	–0.01(4)	2.9(9)	3.0(7)
C123	0.14(3)	–1.5(5)	–1.2(4)
C133	–0.01(1)	–0.8(3)	–0.2(2)
C222	–0.07(2)	0.4(3)	–0.0(3)
C223	–0.02(1)	0.3(3)	–0.1(2)
C233	0.02(1)	0.4(1)	0.0(1)
C333	–0.02(1)	0.0(1)	0.0(1)

Table S3. Fourth order Gram-Charlier coefficients Dijkl scaled by 10^4 for the iodine atom from the POP+CUM refinement.

D1111	0.189(18)
D1112	0.017(18)
D1122	0.131(10)
D1113	0.051(10)
D1123	–0.010(8)
D1133	0.033(3)
D1222	0.032(6)
D1223	0.011(4)
D1233	0.005(2)
D1333	0.004(1)
D2222	0.026(2)
D2223	–0.005(2)
D2233	0.015(1)
D2333	–0.002(1)
D3333	0.003(1)

Table S4. Electronic population parameters from the POP+CUM refinement. P_{core} and P00 are the population values for the first and second monopole functions, respectively. P*lm* (*m*=–*l*, +*l*) indicate dipole (*l*=1), quadrupole (*l*=2), octupole (*l*=3) and hexadecapole (*l*=4) parameters, respectively. The reference Cartesian coordinate system consists of the ***a***, ***a***×***b***×***a***, ***a***×***b*** axes.

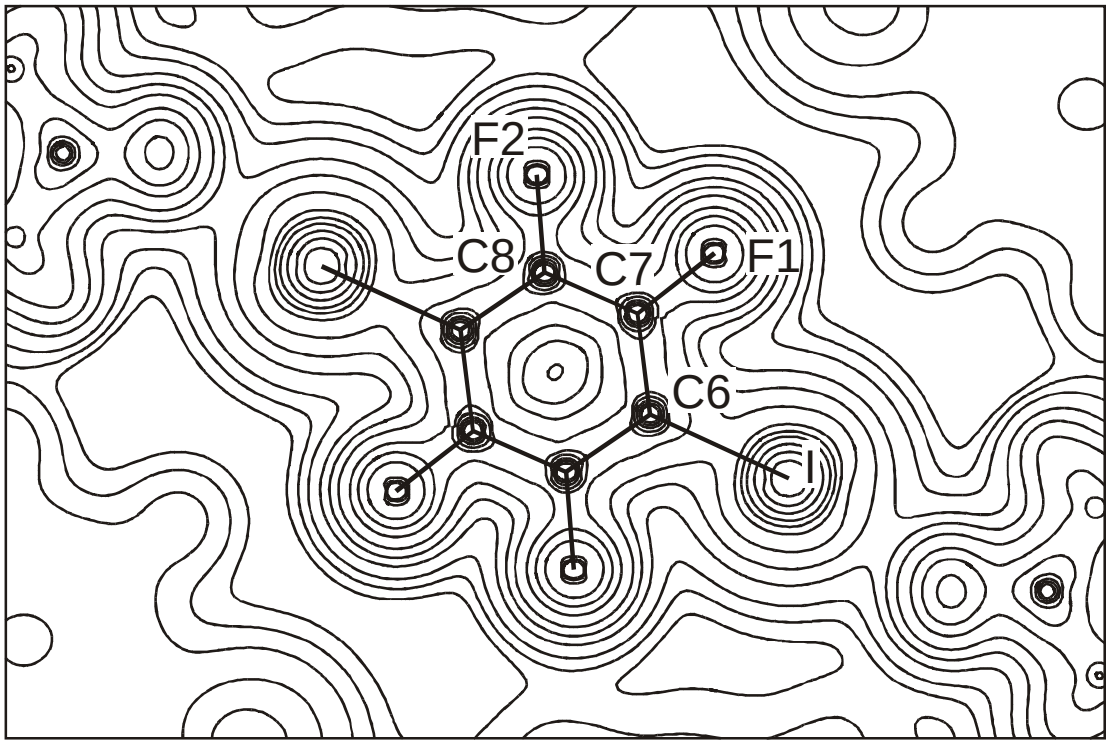
Atom	P_{core}	P00	P11+	P11-	P10
I	47.31(3)	6.18(14)	-0.01(3)	-0.04(3)	0.05(3)
F1	2.039(6)	7.07(4)	0.21(9)	-0.08(7)	-0.03(6)
F2	2.039(6)	7.11(4)	-0.06(8)	-0.02(7)	0.01(5)
O	2.039(6)	6.19(4)	-0.08(2)	-0.09(2)	-0.01(2)
N	2.039(6)	4.89(5)	-0.03(2)	0.02(2)	-0.01(2)
C1	2.039(6)	3.96(8)	0.01(3)	0.01(3)	0.01(3)
C2	2.039(6)	4.05(10)	0.01(3)	-0.04(3)	-0.01(3)
C3	2.039(6)	3.95(7)	-0.05(3)	-0.02(3)	-0.03(3)
C4	2.039(6)	4.05(9)	-0.04(3)	-0.01(3)	0.04(4)
C5	2.039(6)	4.14(9)	-0.02(3)	-0.02(3)	0.03(3)
C6	2.039(6)	3.82(8)	0.01(3)	0.04(3)	0.07(3)
C7	2.039(6)	3.84(8)	-0.03(3)	-0.08(3)	0.00(3)
C8	2.039(6)	3.77(8)	-0.01(3)	-0.08(3)	0.13(3)
H1	-	0.62(6)	0.07(3)	0.01(3)	0.11(4)
H2	-	0.89(9)	-0.02(4)	-0.08(5)	0.12(5)
H4	-	0.93(8)	-0.04(4)	0.01(4)	-0.14(6)
H5	-	0.78(8)	0.06(4)	0.04(4)	-0.07(4)

Atom	P22+	P22-	P21+	P21-	P20
I	0.008(5)	-0.082(10)	-0.040(10)	0.026(11)	-0.078(9)
F1	0.008(4)	-0.027(9)	-0.019(9)	0.012(8)	-0.005(7)
F2	0.003(4)	-0.011(8)	-0.003(8)	0.014(7)	-0.012(6)
O	0.003(4)	-0.025(8)	-0.004(7)	-0.014(7)	0.011(6)
N	-0.005(5)	0.003(9)	-0.005(9)	-0.018(10)	0.013(8)
C1	-0.001(7)	0.040(14)	0.037(13)	-0.004(14)	0.039(12)
C2	-0.004(7)	0.027(14)	0.004(14)	-0.017(15)	0.033(12)
C3	-0.006(6)	0.041(12)	-0.002(13)	-0.044(13)	0.025(12)
C4	-0.007(7)	0.081(14)	0.044(13)	0.034(13)	0.036(13)
C5	-0.002(6)	0.069(14)	-0.005(14)	-0.039(14)	-0.004(12)
C6	-0.017(7)	0.025(14)	-0.005(13)	-0.031(14)	0.003(12)
C7	-0.010(7)	0.019(14)	0.037(14)	-0.017(14)	0.044(13)
C8	-0.016(7)	0.042(15)	-0.005(14)	0.009(14)	0.005(12)

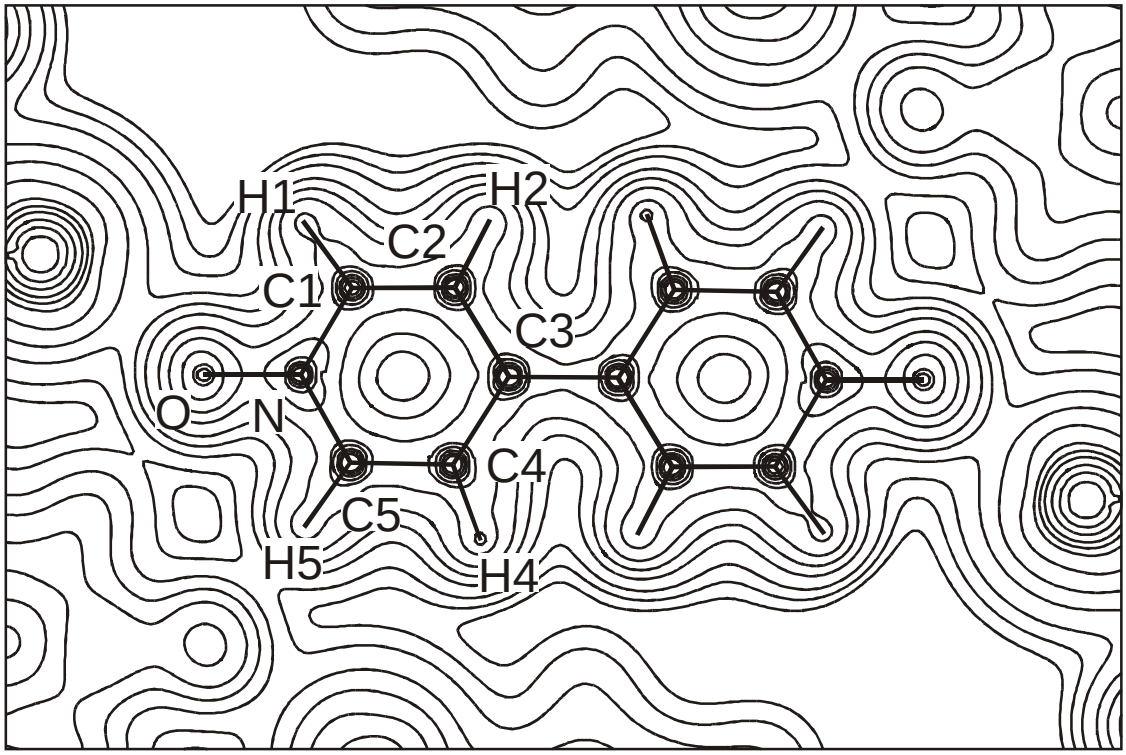
Atom	P33+	P33-	P32+	P32-	P31+	P31-	P30
I	0.0003(7)	-0.0008(7)	-0.0017(16)	-0.0088(32)	0.0004(5)	-0.0006(5)	0.0004(4)
O	-0.0006(8)	0.0017(8)	-0.0031(18)	0.0011(37)	-0.0002(6)	-0.0007(6)	-0.0007(5)
N	0.0011(12)	-0.0029(12)	0.0005(31)	-0.0337(61)	0.0018(10)	0.0008(10)	0.0046(8)
C1	0.0034(21)	0.0024(22)	-0.0182(52)	0.0371(106)	-0.0067(17)	-0.0035(17)	-0.0072(14)
C2	0.0025(21)	-0.0036(21)	0.0064(53)	-0.0450(108)	0.0015(17)	0.0045(18)	0.0065(14)
C3	-0.0027(19)	0.0019(21)	-0.0159(49)	0.0303(102)	-0.0040(17)	-0.0032(19)	-0.0077(13)
C4	-0.0039(21)	-0.0028(21)	-0.0005(50)	-0.0001(101)	0.0108(17)	0.0036(18)	0.0061(14)
C5	0.0012(21)	0.0009(21)	-0.0109(51)	0.0416(105)	-0.0039(17)	-0.0036(17)	-0.0074(14)
C6	0.0031(21)	0.0007(21)	-0.0106(52)	0.0338(102)	0.0002(16)	0.0054(17)	-0.0037(14)
C7	-0.0098(22)	-0.0033(22)	-0.0014(56)	-0.0578(109)	-0.0018(18)	-0.0117(18)	0.0073(15)
C8	0.0006(22)	0.0040(23)	-0.0001(55)	0.0489(107)	0.0005(17)	0.0108(18)	-0.0059(14)

Atom	P44+	P44-	P43+	P43-	P42+	P42-	P41+	P41-	P40
I	0.0014(1)	-0.0008(6)	0.0010(4)	-0.0003(4)	-0.0004(1)	-0.0002(2)	0.0003(1)	0.0003(2)	0.0008(1)

Figure S1. Experimental electron density maps in the same planes of Figure 2. The values of the contours (eÅ^{-3}) increase from the outermost one inwards in steps of 0.15×10^{n}, 0.3×10^{n}, 0.6×10^{n} with n beginning at –1 and increasing in steps of 1.



(*a*)



(*b*)