Electronic Supplementary Material (ESI) for CrystEngComm

SUPPORTING INFORMATION

Structural diversities of charge transfer organic complexes. Focus on benzenoid hydrocarbons and 7,7,8,8-tetracyanoquinodimethane

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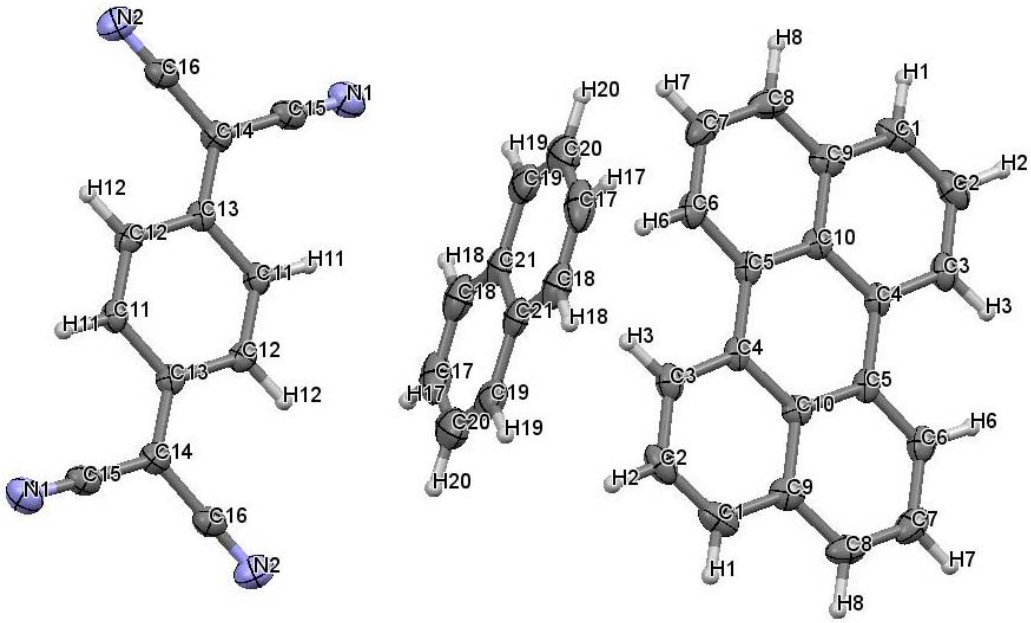


Fig. S1. The molecular structure of (**1**) showing displacement ellipsoid at the 50% probability level.

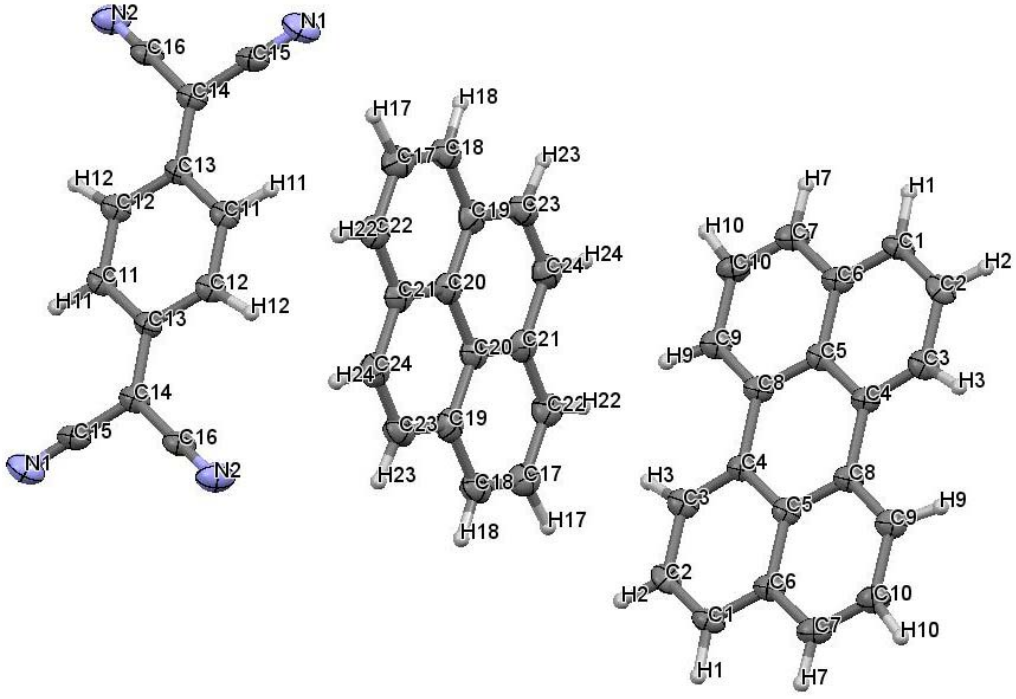


Fig. S2. The molecular structure of (**2**) showing displacement ellipsoid at the 50% probability level.

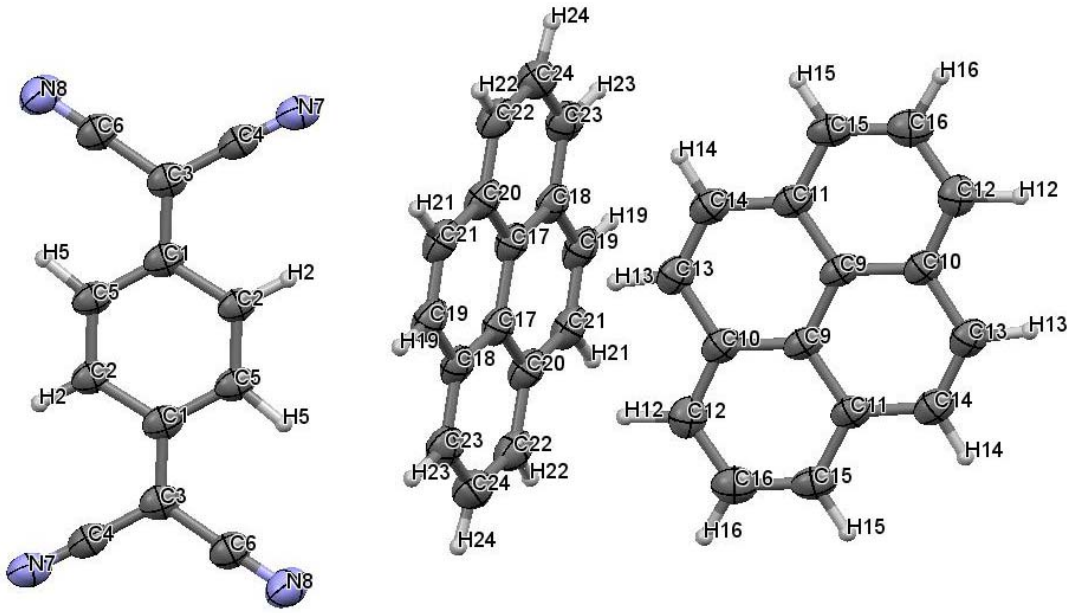


Fig. S3. The molecular structure of (**3**) showing displacement ellipsoid at the 50% probability level.

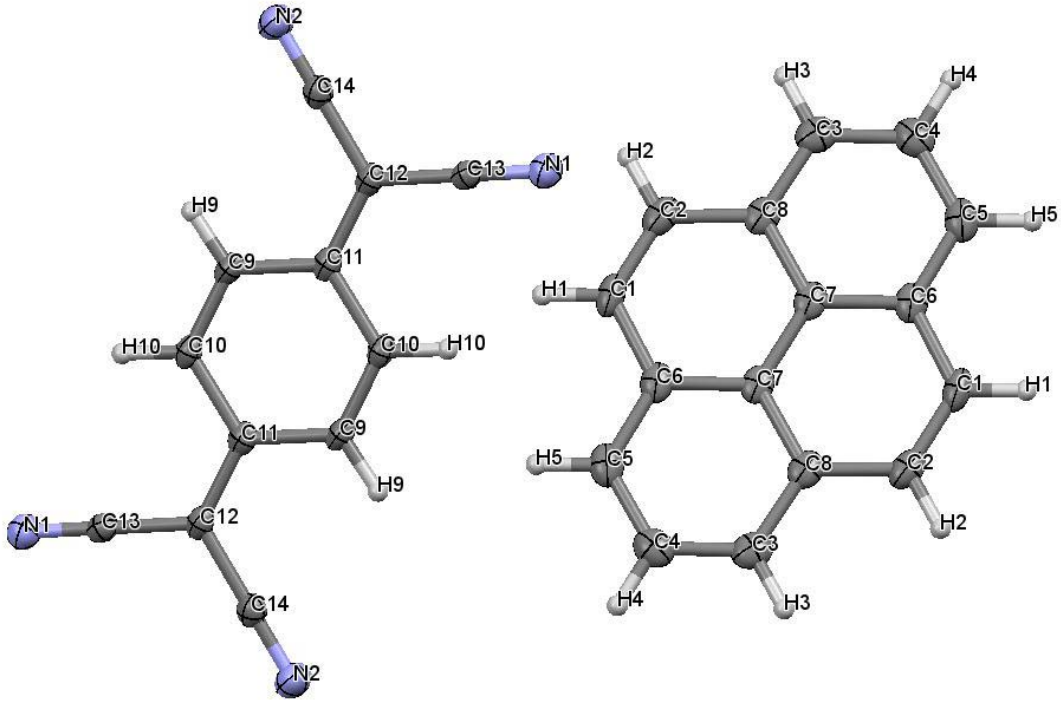


Fig. S4. The molecular structure of (**4**) showing displacement ellipsoid at the 50% probability level.

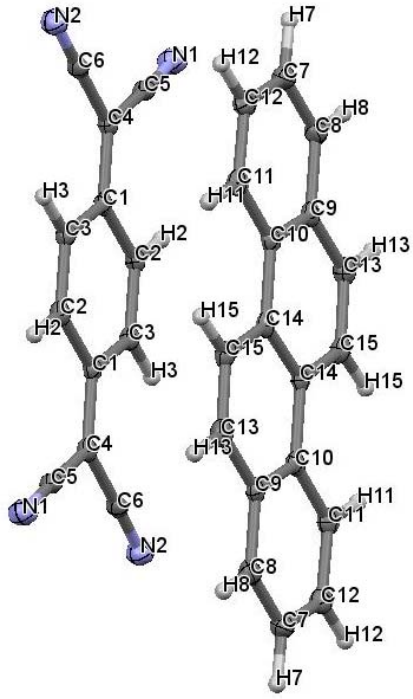


Fig. S5. The molecular structure of (**5**) showing displacement ellipsoid at the 50% probability level.

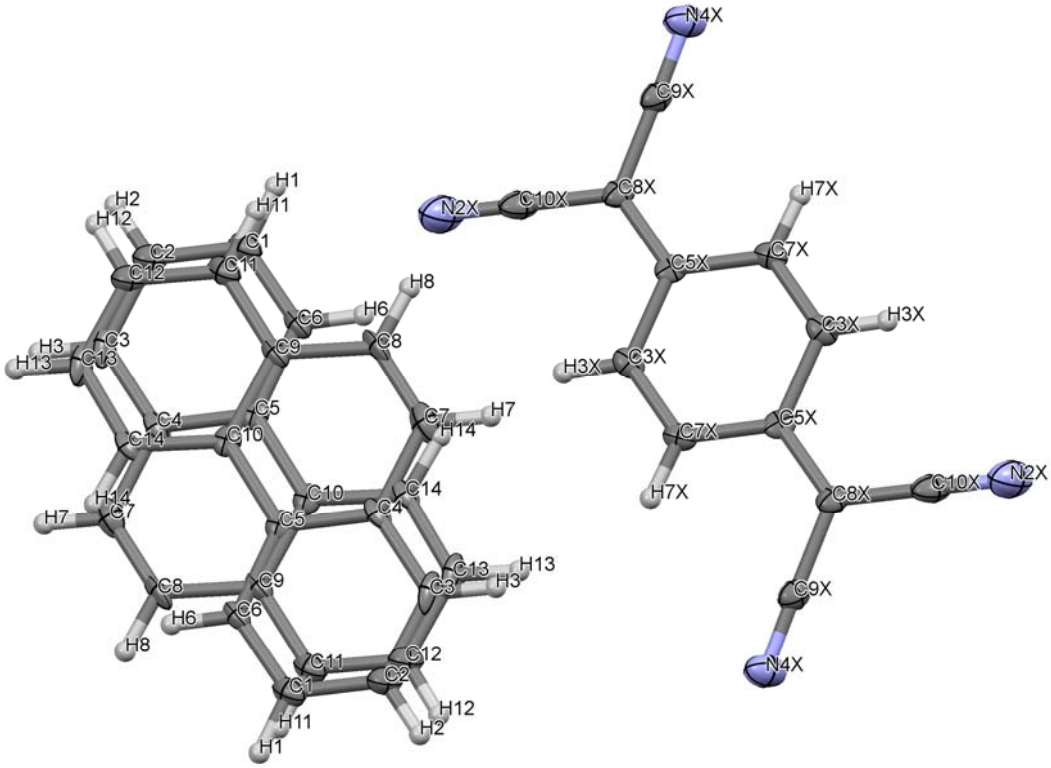


Fig. S6. The molecular structure of (**6**) showing displacement ellipsoid at the 50% probability level.

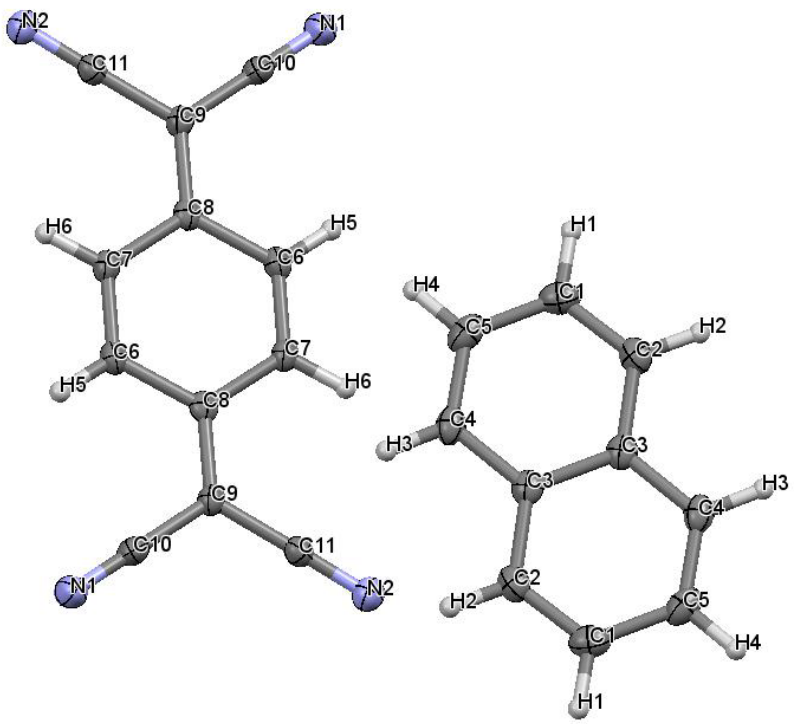
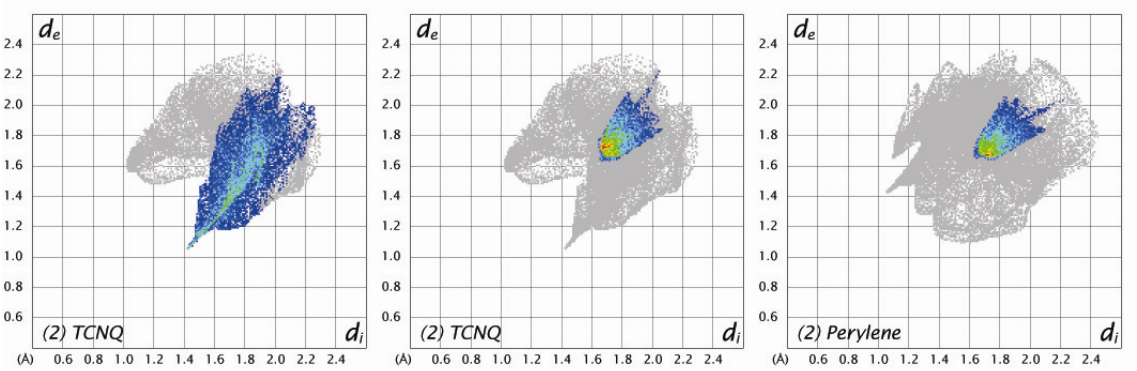
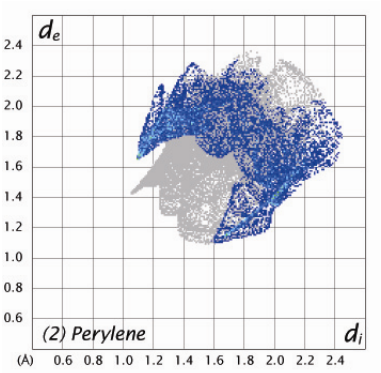


Fig. S7. The molecular structure of (**7**) showing displacement ellipsoid at the 50% probability level.

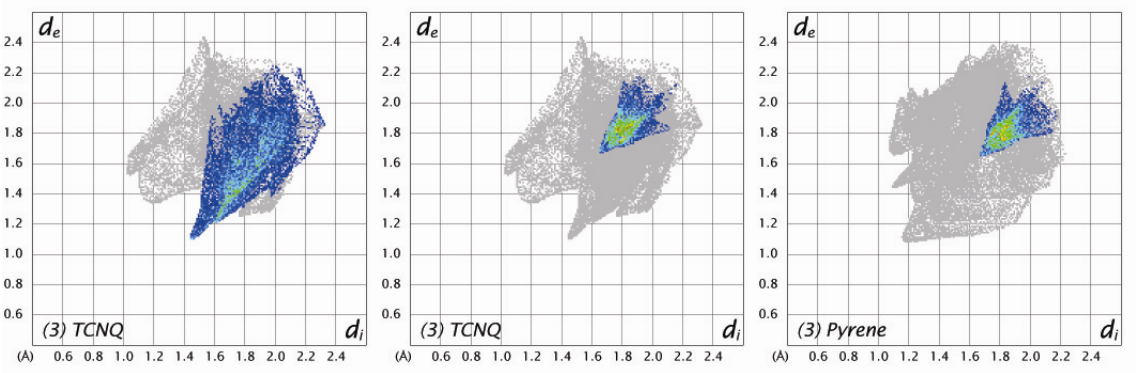


(a) **(b)** **(c)**

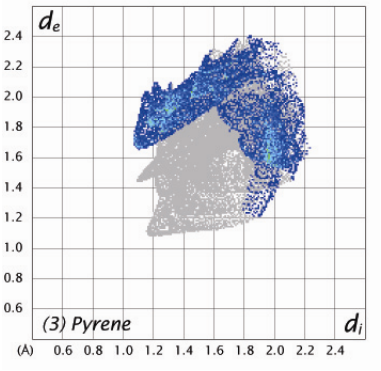


(d)

Fig. S8. Fingerprint plots visualizing d_e and d_i for N···H (**a**), C···C (**b**), (**c**); C-H···π and C···H contacts (**d**) (including reciprocal ones) generated for TCNQ and perylene molecules in complex (**2**).

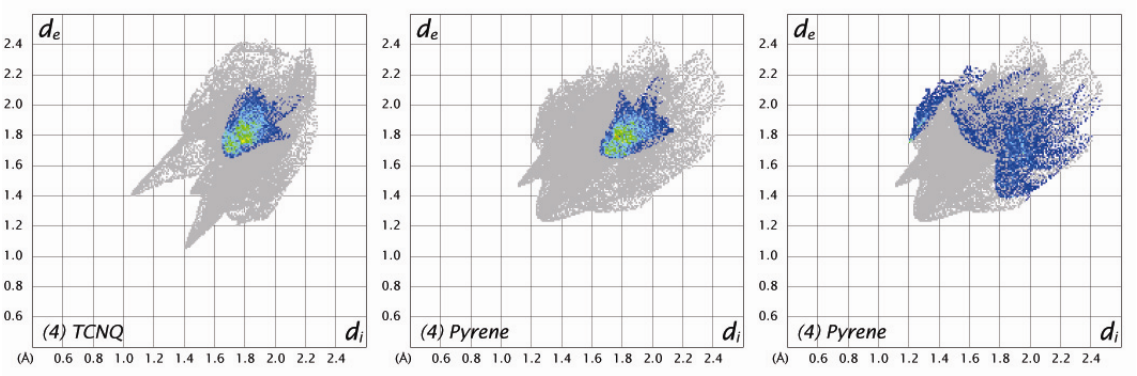


(a) **(b)** **(c)**



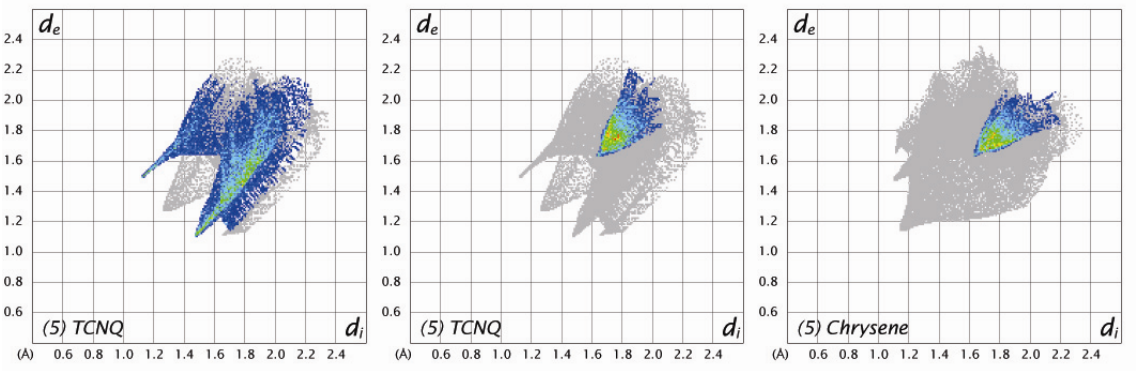
(d)

Fig. S9. Fingerprint plots visualizing d_e and d_i for N···H (**a**) and C···C contacts (**b**), (**c**)); C-H···π and C···H contacts (**d**) (including reciprocal ones) generated for TCNQ and pyrene molecules in complex (**3**).



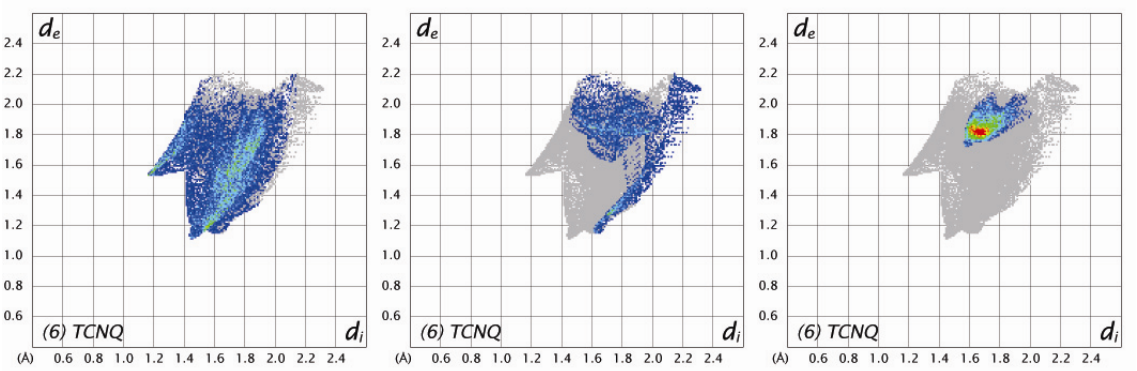
(a) **(b)** **(c)**

Fig. S10. Fingerprint plots visualizing d_e and d_i for C···C (**a**), (**b**) and C···H (**c**) contacts (including reciprocal ones) generated for TCNQ and pyrene molecules in complex (**4**).

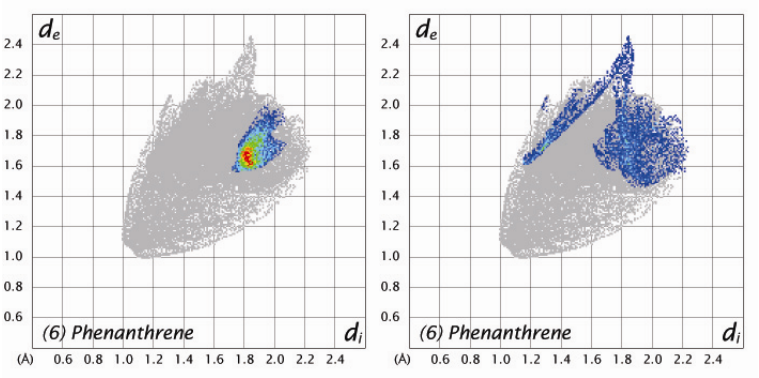


(a) **(b)** **(c)**

Fig. S11. Fingerprint plots visualizing d_e and d_i for N···H (**a**) and C···C contacts (**b**), (**c**) (including reciprocal ones) generated for TCNQ and chrysene molecules in complex (**5**).

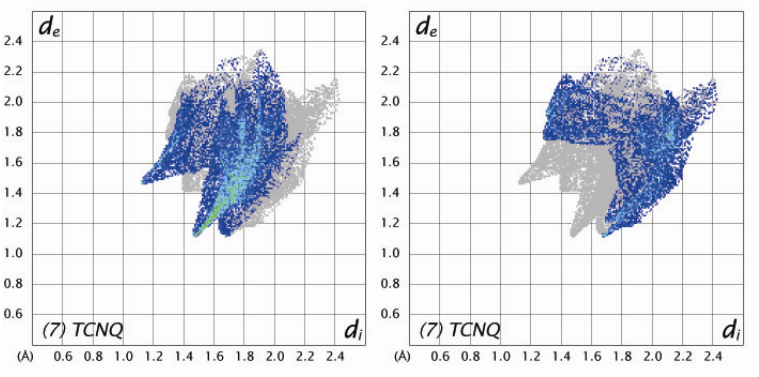


(a) **(b)** **(c)**



(d) **(e)**

Fig. S12. Fingerprint plots visualizing d_e and d_i for N···H (**a**), C···H (**b**), (**e**) and C···C contacts (**c**), (**d**) (including reciprocal ones) generated for TCNQ and phenanthrene molecules in complex (**6**).



(a) **(b)**

Fig. S13. Fingerprint plots visualizing d_e and d_i for N···H (**a**) and C···H contacts (**b**) (including reciprocal ones) generated for TCNQ and naphthalene molecules in complex (**7**).

Table S1. Bond lengths in [Å] for naphthalene-perylene-TCNQ complex (**1**), pyrene-perylene-TCNQ complex (**2**), pyrene-TCNQ (2:1) complex (**3**).

Compound/Parameter	(**1**)	(**2**)		(**3**)	
C(6)-C(7)	1.393(3)	C(4)-C(3)	1.389(5)	C(1)-C(3)	1.379(5)
C(6)-C(5)	1.394(3)	C(4)-C(5)	1.437(4)	C(1)-C(5)	1.412(6)
C(3)-C(4)	1.395(3)	C(4)-C(8)	1.462(4)	C(1)-C(2)	1.445(6)
C(3)-C(2)	1.401(3)	C(3)-C(2)	1.405(5)	C(2)-C(5)#1	1.363(6)
C(13)-C(14)	1.378(3)	C(6)-C(1)	1.414(5)	C(3)-C(4)	1.411(6)
C(13)-C(11)	1.435(3)	C(6)-C(5)	1.422(4)	C(3)-C(6)	1.441(6)
C(13)-C(12)	1.445(3)	C(6)-C(7)	1.427(5)	N(7)-C(4)	1.157(5)
C(10)-C(4)	1.424(3)	C(8)-C(9)	1.398(4)	N(8)-C(6)	1.144(5)
C(10)-C(9)	1.425(3)	C(8)-C(5)#1	1.433(5)	C(9)-C(11)	1.419(6)
C(10)-C(5)	1.432(3)	C(10)-C(7)#1	1.364(5)	C(9)-C(10)	1.427(6)
C(21)-C(19)	1.415(3)	C(10)-C(9)	1.405(5)	C(9)-C(9)#2	1.428(8)
C(21)-C(18)	1.418(3)	C(5)-C(8)#1	1.433(5)	C(10)-C(12)	1.396(6)
C(21)-C(21)#1	1.419(4)	C(2)-C(1)	1.382(5)	C(10)-C(13)	1.430(6)
C(4)-C(5)#2	1.461(3)	C(7)-C(10)#1	1.364(5)	C(11)-C(15)	1.406(6)
C(5)-C(4)#2	1.461(3)	N(1)-C(15)	1.154(4)	C(11)-C(14)	1.434(6)
C(16)-N(2)	1.149(3)	N(2)-C(16)	1.150(4)	C(12)-C(16)	1.397(6)
C(16)-C(14)	1.427(3)	C(13)-C(14)	1.376(4)	C(13)-C(14)#2	1.347(6)
C(8)-C(7)	1.368(3)	C(13)-C(11)	1.436(4)	C(14)-C(13)#2	1.347(6)
C(8)-C(9)	1.411(3)	C(13)-C(12)	1.443(5)	C(15)-C(16)	1.371(6)
C(2)-C(1)	1.366(3)	C(14)-C(15)	1.430(5)	C(17)-C(20)	1.418(6)
C(11)-C(12)#3	1.349(3)	C(14)-C(16)	1.436(5)	C(17)-C(18)	1.422(6)
C(15)-N(1)	1.153(3)	C(12)-C(11)#2	1.358(5)	C(17)-C(17)#3	1.430(8)
C(15)-C(14)	1.432(3)	C(20)-C(21)	1.413(5)	C(18)-C(23)	1.401(6)
C(9)-C(1)	1.415(3)	C(20)-C(19)	1.417(5)	C(18)-C(19)	1.415(6)
C(19)-C(20)	1.349(4)	C(20)-C(20)#3	1.437(7)	C(19)-C(21)	1.355(6)
C(18)-C(17)	1.373(4)	C(19)-C(18)	1.407(5)	C(20)-C(22)	1.385(6)
C(20)-C(17)#1	1.410(4)	C(19)-C(23)	1.434(5)	C(20)-C(21)#3	1.439(6)
		C(21)-C(22)	1.399(5)	C(22)-C(24)	1.389(7)
		C(21)-C(24)	1.446(5)	C(23)-C(24)	1.385(7)
		C(18)-C(17)	1.393(5)		
		C(23)-C(24)#3	1.350(5)		
		C(22)-C(17)	1.385(5)		

Table S2. Bond lengths in [Å] for pyrene-TCNQ (1:1) complex (**4**), chrysene-TCNQ complex (**5**), phenanthrene-TCNQ complex (**6**).

Compound/Parameter	(**4**)	(**5**)		(**6**)	
C(7)-C(8)	1.4218(17)	C(1)-C(4)	1.3803(15)	C(1)-C(2)	1.375(16)
C(7)-C(6)	1.4232(17)	C(1)-C(3)	1.4493(15)	C(1)-C(6)	1.378(14)
C(7)-C(7)#1	1.425(3)	C(1)-C(2)	1.4509(14)	C(2)-C(3)	1.383(16)
C(2)-C(1)	1.346(2)	C(2)-C(3)#1	1.3492(15)	C(3)-C(4)	1.421(16)
C(2)-C(8)	1.4337(18)	C(4)-C(5)	1.4386(14)	C(4)-C(5)	1.411(11)
C(6)-C(5)	1.3955(19)	C(4)-C(6)	1.4394(14)	C(4)-C(7)	1.438(9)
C(6)-C(1)#1	1.4396(18)	C(5)-N(1)	1.1505(14)	C(5)-C(6)	1.408(11)
C(8)-C(3)	1.4011(19)	C(6)-N(2)	1.1509(13)	C(5)-C(10)	1.481(6)
C(3)-C(4)	1.384(2)	C(7)-C(8)	1.3738(16)	C(7)-C(8)	1.324(8)
C(4)-C(5)	1.3861(19)	C(7)-C(12)	1.4041(16)	C(8)-C(9)	1.455(10)
C(10)-C(9)	1.3417(18)	C(8)-C(9)	1.4230(15)	C(9)-C(10)	1.406(11)
C(10)-C(11)	1.4477(16)	C(9)-C(10)	1.4222(15)	C(9)-C(11)	1.425(13)
C(11)-C(12)	1.3747(17)	C(9)-C(13)	1.4274(14)	C(10)-C(14)	1.418(11)
C(11)-C(9)#2	1.4394(16)	C(10)-C(11)	1.4164(15)	C(11)-C(12)	1.380(15)
C(13)-N(1)	1.1498(16)	C(10)-C(14)	1.4569(15)	C(12)-C(13)	1.372(16)
C(13)-C(12)	1.4305(17)	C(11)-C(12)	1.3773(15)	C(13)-C(14)	1.392(16)
C(12)-C(14)	1.4340(17)	C(13)-C(15)#2	1.3625(15)	N(2X)-C(10X)	1.144(4)
C(14)-N(2)	1.1509(16)	C(14)-C(14)#2	1.414(2)	N(4X)-C(9X)	1.144(4)
		C(14)-C(15)	1.4301(15)	C(3X)-C(7X)#1	1.347(4)
				C(3X)-C(5X)	1.446(4)
				C(5X)-C(8X)	1.375(3)
				C(5X)-C(7X)	1.447(4)
				C(7X)-C(3X)#1	1.347(4)
				C(8X)-C(10X)	1.443(4)
				C(8X)-C(9X)	1.450(4)

Table S3. Bond lengths in [Å] for naphthalene-TCNQ complex (**7**).

Compound/Parameter	(**7**)
C(8)-C(9)	1.3741(15)
C(8)-C(7)	1.4430(15)
C(8)-C(6)	1.4449(15)
C(6)-C(7)#1	1.3431(16)
C(11)-N(2)	1.1466(14)
C(11)-C(9)	1.4359(15)
C(3)-C(4)	1.4162(16)
C(3)-C(2)	1.4169(16)
C(3)-C(3)#2	1.423(2)
C(4)-C(5)	1.3616(17)
C(2)-C(1)	1.3642(17)
C(10)-N(1)	1.1499(15)
C(10)-C(9)	1.4322(15)
C(5)-C(1)#2	1.4115(17)

Table S4. Bond angles [°] for naphthalene-perylene-TCNQ complex (**1**), pyrene-perylene-TCNQ complex (**2**), pyrene-TCNQ (2:1) complex (**3**).

Compound/Parameter	(**1**)	(**2**)		(**3**)	
C(7)-C(6)-C(5)	122.1(2)	C(3)-C(4)-C(5)	118.3(3)	C(3)-C(1)-C(5)	121.9(4)
C(4)-C(3)-C(2)	121.6(2)	C(3)-C(4)-C(8)	121.9(3)	C(3)-C(1)-C(2)	119.1(4)
C(14)-C(13)-C(11)	121.06(18)	C(5)-C(4)-C(8)	119.8(3)	C(5)-C(1)-C(2)	119.1(4)
C(14)-C(13)-C(12)	121.35(18)	C(4)-C(3)-C(2)	121.9(3)	C(5)#1-C(2)-C(1)	119.9(4)
C(11)-C(13)-C(12)	117.58(18)	C(1)-C(6)-C(5)	120.2(3)	C(1)-C(3)-C(4)	122.1(4)
C(4)-C(10)-C(9)	119.59(18)	C(1)-C(6)-C(7)	120.2(3)	C(1)-C(3)-C(6)	121.2(4)
C(4)-C(10)-C(5)	121.20(18)	C(5)-C(6)-C(7)	119.6(3)	C(4)-C(3)-C(6)	116.7(4)
C(9)-C(10)-C(5)	119.21(18)	C(9)-C(8)-C(5)#1	118.6(3)	C(2)#1-C(5)-C(1)	121.0(4)
C(19)-C(21)-C(18)	121.8(2)	C(9)-C(8)-C(4)	122.4(3)	N(7)-C(4)-C(3)	177.9(4)
C(19)-C(21)-C(21)#1	119.6(3)	C(5)#1-C(8)-C(4)	119.0(3)	N(8)-C(6)-C(3)	178.3(5)
C(18)-C(21)-C(21)#1	118.6(3)	C(7)#1-C(10)-C(9)	120.7(3)	C(11)-C(9)-C(10)	120.4(4)
C(3)-C(4)-C(10)	118.38(19)	C(6)-C(5)-C(8)#1	119.4(3)	C(11)-C(9)-C(9)#2	119.8(5)
C(3)-C(4)-C(5)#2	122.27(19)	C(6)-C(5)-C(4)	119.4(3)	C(10)-C(9)-C(9)#2	119.8(4)
C(10)-C(4)-C(5)#2	119.35(17)	C(8)#1-C(5)-C(4)	121.2(3)	C(12)-C(10)-C(9)	118.6(4)
C(6)-C(5)-C(10)	118.23(19)	C(8)-C(9)-C(10)	121.5(3)	C(12)-C(10)-C(13)	122.7(4)
C(6)-C(5)-C(4)#2	122.33(18)	C(1)-C(2)-C(3)	120.4(3)	C(9)-C(10)-C(13)	118.6(4)
C(10)-C(5)-C(4)#2	119.44(17)	C(2)-C(1)-C(6)	119.7(3)	C(15)-C(11)-C(9)	118.6(4)
N(2)-C(16)-C(14)	178.5(2)	C(10)#1-C(7)-C(6)	120.2(3)	C(15)-C(11)-C(14)	122.7(4)
C(7)-C(8)-C(9)	120.6(2)	C(14)-C(13)-C(11)	121.7(3)	C(9)-C(11)-C(14)	118.7(4)
C(8)-C(7)-C(6)	120.2(2)	C(14)-C(13)-C(12)	120.4(3)	C(10)-C(12)-C(16)	120.6(4)
C(1)-C(2)-C(3)	120.7(2)	C(11)-C(13)-C(12)	117.9(3)	C(14)#2-C(13)-C(10)	121.4(4)
C(12)#3-C(11)-C(13)	121.47(19)	C(13)-C(14)-C(15)	121.8(3)	C(13)#2-C(14)-C(11)	121.6(4)
C(11)#3-C(12)-C(13)	120.94(19)	C(13)-C(14)-C(16)	122.6(3)	C(16)-C(15)-C(11)	120.9(4)
N(1)-C(15)-C(14)	177.8(2)	C(15)-C(14)-C(16)	115.6(3)	C(15)-C(16)-C(12)	121.0(4)
C(8)-C(9)-C(1)	120.7(2)	C(11)#2-C(12)-C(13)	120.7(3)	C(20)-C(17)-C(18)	120.4(4)
C(8)-C(9)-C(10)	119.7(2)	C(12)#2-C(11)-C(13)	121.4(3)	C(20)-C(17)-C(17)#3	120.5(5)
C(1)-C(9)-C(10)	119.6(2)	N(1)-C(15)-C(14)	179.3(4)	C(18)-C(17)-C(17)#3	119.1(5)
C(13)-C(14)-C(16)	121.72(19)	N(2)-C(16)-C(14)	178.1(3)	C(23)-C(18)-C(19)	123.2(4)
C(13)-C(14)-C(15)	120.91(19)	C(21)-C(20)-C(19)	120.3(3)	C(23)-C(18)-C(17)	117.8(4)
C(16)-C(14)-C(15)	117.37(18)	C(21)-C(20)-C(20)#3	120.1(4)	C(19)-C(18)-C(17)	119.0(4)
C(2)-C(1)-C(9)	120.1(2)	C(19)-C(20)-C(20)#3	119.6(4)	C(21)-C(19)-C(18)	122.4(4)
C(20)-C(19)-C(21)	120.5(3)	C(18)-C(19)-C(20)	119.1(3)	C(22)-C(20)-C(17)	119.2(4)
C(17)-C(18)-C(21)	120.0(2)	C(18)-C(19)-C(23)	121.7(3)	C(22)-C(20)-C(21)#3	122.2(4)
C(19)-C(20)-C(17)#1	120.5(3)	C(20)-C(19)-C(23)	119.2(3)	C(17)-C(20)-C(21)#3	118.6(4)
C(18)-C(17)-C(20)#1	120.8(3)	C(22)-C(21)-C(20)	119.0(3)	C(19)-C(21)-C(20)#3	120.4(4)
		C(22)-C(21)-C(24)	122.6(3)	C(20)-C(22)-C(24)	121.1(5)
		C(20)-C(21)-C(24)	118.4(3)	C(24)-C(23)-C(18)	121.7(4)
		C(17)-C(18)-C(19)	120.0(3)	C(23)-C(24)-C(22)	119.8(5)
		C(24)#3-C(23)-C(19)	121.1(3)		
		C(23)#3-C(24)-C(21)	121.5(3)		
		C(17)-C(22)-C(21)	120.8(3)		
		C(22)-C(17)-C(18)	120.8(3)		

Table S5. Bond angles [°] for pyrene-TCNQ (1:1) complex (**4**), chrysene-TCNQ complex (**5**), phenanthrene-TCNQ complex (**6**).

Compound/Parameter	(**4**)	(**5**)		(**6**)	
C(8)-C(7)-C(6)	120.00(12)	C(4)-C(1)-C(3)	120.81(9)	C(2)-C(1)-C(6)	120.3(9)
C(8)-C(7)-C(7)#1	120.06(14)	C(4)-C(1)-C(2)	120.99(9)	C(1)-C(2)-C(3)	121.1(11)
C(6)-C(7)-C(7)#1	119.94(14)	C(3)-C(1)-C(2)	118.20(9)	C(2)-C(3)-C(4)	119.9(10)
C(1)-C(2)-C(8)	121.29(12)	C(3)#1-C(2)-C(1)	120.46(10)	C(5)-C(4)-C(3)	118.6(8)
C(5)-C(6)-C(7)	118.91(12)	C(2)#1-C(3)-C(1)	121.33(10)	C(5)-C(4)-C(7)	121.1(8)
C(5)-C(6)-C(1)#1	122.81(12)	C(1)-C(4)-C(5)	122.94(9)	C(3)-C(4)-C(7)	120.3(9)
C(7)-C(6)-C(1)#1	118.28(12)	C(1)-C(4)-C(6)	121.79(9)	C(6)-C(5)-C(4)	119.5(9)
C(3)-C(8)-C(7)	118.87(12)	C(5)-C(4)-C(6)	115.28(9)	C(6)-C(5)-C(10)	122.9(8)
C(3)-C(8)-C(2)	122.42(12)	N(1)-C(5)-C(4)	177.67(10)	C(4)-C(5)-C(10)	117.6(7)
C(7)-C(8)-C(2)	118.69(12)	N(2)-C(6)-C(4)	179.22(11)	C(1)-C(6)-C(5)	120.5(9)
C(2)-C(1)-C(6)#1	121.72(12)	C(8)-C(7)-C(12)	120.09(10)	C(8)-C(7)-C(4)	120.8(6)
C(4)-C(3)-C(8)	120.59(12)	C(7)-C(8)-C(9)	120.37(10)	C(7)-C(8)-C(9)	121.8(6)
C(3)-C(4)-C(5)	120.88(13)	C(10)-C(9)-C(8)	119.67(10)	C(10)-C(9)-C(11)	119.3(9)
C(4)-C(5)-C(6)	120.75(12)	C(10)-C(9)-C(13)	119.35(10)	C(10)-C(9)-C(8)	119.2(8)
C(9)-C(10)-C(11)	120.93(11)	C(8)-C(9)-C(13)	120.98(10)	C(11)-C(9)-C(8)	121.4(8)
C(12)-C(11)-C(9)#2	121.56(10)	C(11)-C(10)-C(9)	118.23(10)	C(9)-C(10)-C(14)	118.5(9)
C(12)-C(11)-C(10)	120.32(10)	C(11)-C(10)-C(14)	122.85(10)	C(9)-C(10)-C(5)	119.5(7)
C(9)#2-C(11)-C(10)	118.12(11)	C(9)-C(10)-C(14)	118.92(10)	C(14)-C(10)-C(5)	122.0(7)
N(1)-C(13)-C(12)	179.91(17)	C(12)-C(11)-C(10)	120.89(10)	C(12)-C(11)-C(9)	120.3(9)
C(10)-C(9)-C(11)#2	120.95(11)	C(11)-C(12)-C(7)	120.73(10)	C(13)-C(12)-C(11)	120.8(11)
C(11)-C(12)-C(13)	121.66(10)	C(15)#2-C(13)-C(9)	121.53(10)	C(12)-C(13)-C(14)	120.4(11)
C(11)-C(12)-C(14)	122.20(10)	C(14)#2-C(14)-C(15)	119.28(12)	C(13)-C(14)-C(10)	120.7(9)
C(13)-C(12)-C(14)	116.12(11)	C(14)#2-C(14)-C(10)	119.81(12)	C(7X)#1-C(3X)-C(5X)	121.1(3)
N(2)-C(14)-C(12)	178.70(12)	C(15)-C(14)-C(10)	120.91(9)	C(8X)-C(5X)-C(3X)	120.8(3)
		C(13)#2-C(15)-C(14)	121.11(10)	C(8X)-C(5X)-C(7X)	120.8(3)
				C(3X)-C(5X)-C(7X)	118.4(2)
				C(3X)#1-C(7X)-C(5X)	120.4(3)
				C(5X)-C(8X)-C(10X)	121.7(3)
				C(5X)-C(8X)-C(9X)	123.4(3)
				C(10X)-C(8X)-C(9X)	114.9(3)
				N(4X)-C(9X)-C(8X)	178.8(3)
				N(2X)-C(10X)-C(8X)	179.6(3)

Table S6. Bond lengths [°] for naphthalene-TCNQ complex (**7**).

Compound/Parameter	(**7**)
C(9)-C(8)-C(7)	121.09(10)
C(9)-C(8)-C(6)	120.72(10)
C(7)-C(8)-C(6)	118.19(10)
C(6)#1-C(7)-C(8)	121.05(10)
N(2)-C(11)-C(9)	178.72(11)
C(7)#1-C(6)-C(8)	120.76(10)
C(4)-C(3)-C(2)	122.14(10)
C(4)-C(3)-C(3)#2	118.80(13)
C(2)-C(3)-C(3)#2	119.06(13)
C(5)-C(4)-C(3)	120.78(11)
C(1)-C(2)-C(3)	120.45(11)
N(1)-C(10)-C(9)	178.53(12)
C(8)-C(9)-C(10)	122.02(10)
C(8)-C(9)-C(11)	122.64(9)
C(10)-C(9)-C(11)	115.31(9)
C(4)-C(5)-C(1)#2	120.38(11)
C(2)-C(1)-C(5)#2	120.53(11)

Table S7. Torsion angles [°] for naphthalene-perylene-TCNQ complex (**1**), pyrene-perylene-TCNQ complex (**2**), pyrene-TCNQ (2:1) complex (**3**).

Compound/Parameter	(**1**)	(**2**)		(**3**)	
C(2)-C(3)-C(4)-C(10)	-1.3(3)	C(5)-C(4)-C(3)-C(2)	-1.9(5)	C(3)-C(1)-C(2)-C(5)#1	179.7(3)
C(2)-C(3)-C(4)-C(5)#2	178.95(2)	C(8)-C(4)-C(3)-C(2)	179.0(3)	C(5)-C(1)-C(2)-C(5)#1	0.6(6)
C(9)-C(10)-C(4)-C(3)	1.1(3)	C(3)-C(4)-C(8)-C(9)	-1.6(5)	C(5)-C(1)-C(3)-C(4)	-178.8(3)
C(5)-C(10)-C(4)-C(3)	-178.58(2)	C(5)-C(4)-C(8)-C(9)	179.2(3)	C(2)-C(1)-C(3)-C(4)	2.1(5)
C(9)-C(10)-C(4)-C(5)#2	-179.23(2)	C(3)-C(4)-C(8)-C(5)#1	178.4(3)	C(5)-C(1)-C(3)-C(6)	1.4(6)
C(5)-C(10)-C(4)-C(5)#2	1.1(3)	C(5)-C(4)-C(8)-C(5)#1	-0.8(5)	C(2)-C(1)-C(3)-C(6)	-177.7(4)
C(7)-C(6)-C(5)-C(10)	1.6(3)	C(1)-C(6)-C(5)-C(8)#1	179.8(3)	C(3)-C(1)-C(5)-C(2)#1	-179.7(4)
C(7)-C(6)-C(5)-C(4)#2	-178.94(2)	C(7)-C(6)-C(5)-C(8)#1	0.0(4)	C(11)-C(9)-C(10)-C(12)	0.3(5)
C(4)-C(10)-C(5)-C(6)	178.32(2)	C(1)-C(6)-C(5)-C(4)	0.2(4)	C(11)-C(9)-C(10)-C(13)	179.7(3)
C(9)-C(10)-C(5)-C(6)	-1.3(3)	C(7)-C(6)-C(5)-C(4)	-179.7(3)	C(10)-C(9)-C(11)-C(15)	-0.8(5)
C(4)-C(10)-C(5)-C(4)#2	-1.1(3)	C(3)-C(4)-C(5)-C(6)	1.2(4)	C(10)-C(9)-C(11)-C(14)	179.7(3)
C(9)-C(10)-C(5)-C(4)#2	179.22(2)	C(8)-C(4)-C(5)-C(6)	-179.6(2)	C(9)-C(10)-C(12)-C(16)	0.3(6)
C(9)-C(8)-C(7)-C(6)	-0.7(3)	C(3)-C(4)-C(5)-C(8)#1	-178.4(3)	C(13)-C(10)-C(12)-C(16)	-179.1(4)
C(5)-C(6)-C(7)-C(8)	-0.6(3)	C(8)-C(4)-C(5)-C(8)#1	0.8(5)	C(9)-C(11)-C(15)-C(16)	0.7(6)
C(4)-C(3)-C(2)-C(1)	0.0(3)	C(5)#1-C(8)-C(9)-C(10)	-0.4(5)	C(14)-C(11)-C(15)-C(16)	-179.7(4)
C(14)-C(13)-C(11)-C(12)#3	179.97(2)	C(4)-C(8)-C(9)-C(10)	179.6(3)	C(11)-C(15)-C(16)-C(12)	-0.2(6)
C(12)-C(13)-C(11)-C(12)#3	0.4(3)	C(4)-C(3)-C(2)-C(1)	1.1(5)	C(10)-C(12)-C(16)-C(15)	-0.3(6)
C(14)-C(13)-C(12)-C(11)#3	-179.96(2)	C(3)-C(2)-C(1)-C(6)	0.3(5)	C(20)-C(17)-C(18)-C(23)	-1.3(6)
C(11)-C(13)-C(12)-C(11)#3	-0.4(3)	C(5)-C(6)-C(1)-C(2)	-1.0(5)	C(20)-C(17)-C(18)-C(19)	-180.0(3)
C(7)-C(8)-C(9)-C(1)	-179.10(2)	C(7)-C(6)-C(1)-C(2)	178.9(3)	C(23)-C(18)-C(19)-C(21)	-179.0(4)
C(7)-C(8)-C(9)-C(10)	1.0(3)	C(1)-C(6)-C(7)-C(10)#1	-179.3(3)	C(18)-C(17)-C(20)-C(22)	0.6(6)
C(4)-C(10)-C(9)-C(8)	-179.57(2)	C(5)-C(6)-C(7)-C(10)#1	0.5(5)	C(17)-C(20)-C(22)-C(24)	0.1(6)
C(5)-C(10)-C(9)-C(8)	0.1(3)	C(11)-C(13)-C(14)-C(15)	-0.6(5)	C(19)-C(18)-C(23)-C(24)	179.8(4)
C(4)-C(10)-C(9)-C(1)	0.5(3)	C(12)-C(13)-C(14)-C(15)	178.9(3)	C(17)-C(18)-C(23)-C(24)	1.2(6)
C(5)-C(10)-C(9)-C(1)	-179.87(2)	C(11)-C(13)-C(14)-C(16)	179.1(3)	C(18)-C(23)-C(24)-C(22)	-0.5(7)
C(11)-C(13)-C(14)-C(16)	-179.60(2)	C(12)-C(13)-C(14)-C(16)	-1.4(5)	C(20)-C(22)-C(24)-C(23)	-0.2(7)
N(2)-C(16)-C(14)-C(13)	17(9)	C(13)-C(14)-C(15)-N(1)	-177(1)	C(1)-C(3)-C(4)-N(7)	34(1)
N(2)-C(16)-C(14)-C(15)	-163(9)	C(16)-C(14)-C(15)-N(1)	3(31)	C(6)-C(3)-C(4)-N(7)	-146(1)
N(1)-C(15)-C(14)-C(13)	3(6)	C(13)-C(14)-C(16)-N(2)	-49(1)	C(1)-C(3)-C(6)-N(8)	35(2)
N(1)-C(15)-C(14)-C(16)	-177(1)	C(15)-C(14)-C(16)-N(2)	131(1)	C(4)-C(3)-C(6)-N(8)	-144(2)
C(3)-C(2)-C(1)-C(9)	1.6(3)	C(21)-C(20)-C(19)-C(18)	0.8(5)		
C(8)-C(9)-C(1)-C(2)	178.24(2)	C(21)-C(20)-C(19)-C(23)	-179.1(3)		
C(10)-C(9)-C(1)-C(2)	-1.8(3)	C(20)-C(19)-C(18)-C(17)	-1.1(5)		
		C(23)-C(19)-C(18)-C(17)	178.8(3)		
		C(24)-C(21)-C(22)-C(17)	178.7(3)		

Table S8. Torsion angles [°] for pyrene-TCNQ (1:1) complex (**4**), chrysene-TCNQ complex (**5**), phenanthrene-TCNQ complex (**6**).

Compound/Parameter	(**4**)	(**5**)		(**6**)	
C(8)-C(7)-C(6)-C(5)	-0.08(2)	C(4)-C(1)-C(2)-C(3)#1	179.75(9)	C(6)-C(1)-C(2)-C(3)	-0.4(5)
C(7)#1-C(7)-C(6)-C(5)	179.77(1)	C(3)-C(1)-C(2)-C(3)#1	-0.23(2)	C(1)-C(2)-C(3)-C(4)	-0.1(4)
C(8)-C(7)-C(6)-C(1)#1	179.15(1)	C(3)-C(1)-C(4)-C(5)	179.58(8)	C(2)-C(3)-C(4)-C(5)	0.0(9)
C(7)#1-C(7)-C(6)-C(1)#1	-1.01(2)	C(2)-C(1)-C(4)-C(5)	-0.40(2)	C(2)-C(3)-C(4)-C(7)	179.5(5)
C(6)-C(7)-C(8)-C(3)	0.58(2)	C(3)-C(1)-C(4)-C(6)	-1.16(2)	C(3)-C(4)-C(5)-C(6)	0.5(12)
C(7)#1-C(7)-C(8)-C(3)	-179.27(1)	C(2)-C(1)-C(4)-C(6)	178.86(8)	C(7)-C(4)-C(5)-C(6)	-178.9(7)
C(6)-C(7)-C(8)-C(2)	179.17(1)	C(12)-C(7)-C(8)-C(9)	0.81(2)	C(3)-C(4)-C(5)-C(10)	179.8(5)
C(7)#1-C(7)-C(8)-C(2)	-0.67(2)	C(7)-C(8)-C(9)-C(10)	-0.80(2)	C(7)-C(4)-C(5)-C(10)	0.4(9)
C(1)-C(2)-C(8)-C(3)	179.18(1)	C(7)-C(8)-C(9)-C(13)	179.01(9)	C(2)-C(1)-C(6)-C(5)	0.9(10)
C(1)-C(2)-C(8)-C(7)	0.63(2)	C(8)-C(9)-C(10)-C(11)	-0.01(1)	C(4)-C(5)-C(6)-C(1)	-1.0(13)
C(8)-C(2)-C(1)-C(6)#1	0.25(2)	C(13)-C(9)-C(10)-C(11)	-179.82(8)	C(10)-C(5)-C(6)-C(1)	179.8(5)
C(7)-C(8)-C(3)-C(4)	-0.60(2)	C(8)-C(9)-C(10)-C(14)	-179.85(8)	C(5)-C(4)-C(7)-C(8)	-0.3(10)
C(2)-C(8)-C(3)-C(4)	-179.15(1)	C(13)-C(9)-C(10)-C(14)	0.34(1)	C(3)-C(4)-C(7)-C(8)	-179.8(5)
C(8)-C(3)-C(4)-C(5)	0.13(2)	C(9)-C(10)-C(11)-C(12)	0.81(2)	C(4)-C(7)-C(8)-C(9)	-0.4(8)
C(3)-C(4)-C(5)-C(6)	0.39(2)	C(14)-C(10)-C(11)-C(12)	-179.36(9)	C(7)-C(8)-C(9)-C(10)	1.1(10)
C(7)-C(6)-C(5)-C(4)	-0.41(2)	C(10)-C(11)-C(12)-C(7)	-0.82(2)	C(7)-C(8)-C(9)-C(11)	-179.5(6)
C(1)#1-C(6)-C(5)-C(4)	-179.60(1)	C(8)-C(7)-C(12)-C(11)	-0.01(2)	C(11)-C(9)-C(10)-C(14)	0.2(12)
C(9)-C(10)-C(11)-C(12)	179.26(1)	C(10)-C(9)-C(13)-C(15)#2	0.62(2)	C(8)-C(9)-C(10)-C(14)	179.6(7)
C(9)-C(10)-C(11)-C(9)#2	-0.24(2)	C(8)-C(9)-C(13)-C(15)#2	-179.20(9)	C(11)-C(9)-C(10)-C(5)	179.6(6)
C(11)-C(10)-C(9)-C(11)#2	0.25(2)	C(11)-C(10)-C(14)-C(14)#2	179.39(1)	C(8)-C(9)-C(10)-C(5)	-1.0(10)
C(9)#2-C(11)-C(12)-C(13)	-179.46(1)	C(9)-C(10)-C(14)-C(14)#2	-0.77(2)	C(6)-C(5)-C(10)-C(9)	179.6(1)
C(10)-C(11)-C(12)-C(13)	1.06(2)	C(11)-C(10)-C(14)-C(15)	-0.32(2)	C(10)-C(9)-C(11)-C(12)	1.0(1)
C(9)#2-C(11)-C(12)-C(14)	2.21(2)	C(9)-C(10)-C(14)-C(15)	179.52(8)	C(11)-C(12)-C(13)-C(14)	-0.2(9)
C(10)-C(11)-C(12)-C(14)	-177.27(1)	C(14)#2-C(14)-C(15)-C(13)#2	-0.67(2)	C(5)-C(10)-C(14)-C(13)	179.2(5)
N(1)-C(13)-C(12)-C(11)	-150(1)	C(1)-C(4)-C(5)-N(1)	-177(1)	C(5X)-C(8X)-C(9X)-N(4X)	-134(2)
N(1)-C(13)-C(12)-C(14)	29(1)	C(6)-C(4)-C(5)-N(1)	3(3)	C(10X)-C(8X)-C(9X)-N(4X)	46(2)
C(11)-C(12)-C(14)-N(2)	98(6)	C(1)-C(4)-C(6)-N(2)	-130(8)	C(5X)-C(8X)-C(10X)-N(2X)	-82(6)
C(13)-C(12)-C(14)-N(2)	-80(6)	C(5)-C(4)-C(6)-N(2)	50(8)	C(9X)-C(8X)-C(10X)-N(2X)	99(6)

Table S9. Torsion angles [°] for naphthalene-TCNQ complex (**7**).

Compound/Parameter	(**7**)
C(9)-C(8)-C(7)-C(6)#1	-178.21(10)
C(6)-C(8)-C(7)-C(6)#1	0.81(16)
C(9)-C(8)-C(6)-C(7)#1	178.21(9)
C(7)-C(8)-C(6)-C(7)#1	-0.81(16)
C(2)-C(3)-C(4)-C(5)	-179.68(10)
C(3)#2-C(3)-C(4)-C(5)	0.21(19)
C(4)-C(3)-C(2)-C(1)	-179.97(10)
C(3)#2-C(3)-C(2)-C(1)	0.14(18)
C(7)-C(8)-C(9)-C(10)	176.41(9)
C(6)-C(8)-C(9)-C(10)	-2.58(16)
C(7)-C(8)-C(9)-C(11)	-1.44(16)
C(6)-C(8)-C(9)-C(11)	179.57(9)
C(3)-C(4)-C(5)-C(1)#2	-0.49(17)
C(3)-C(2)-C(1)-C(5)#2	0.13(17)
N(1)-C(10)-C(9)-C(8)	-102(4)
N(1)-C(10)-C(9)-C(11)	76(4)
N(2)-C(11)-C(9)-C(8)	162(5)
N(2)-C(11)-C(9)-C(10)	-16(5)