Electronic Supporting Information

Organic–Inorganic {d_z^2-$M^{II}S_4$}···π-Hole Stacking in Reverse Sandwich Structures. The Case of Cocrystals of Group 10 Metal Dithiocarbamates with Electron-deficient Arenes

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Crystallographic data

Table S1. Crystallographic data and structure refinement for (**1**–**3**)·2(FXB)

Identification code	2154457	2154459	2154460	2154461
Empirical formula	$C_{22}H_{20}F_8I_4N_2NiS_4$	$C_{22}H_{20}Br_4F_8N_2NiS_4$	$C_{22}H_{20}Br_4F_8N_2PdS_4$	$C_{22}H_{20}Br_4F_8N_2PtS_4$
Formula weight	1158.95	970.99	1018.68	1107.37
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1	P-1
a/Å	9.0182(4)	8.74100(10)	8.7298(4)	8.7387(4)
b/Å	9.8168(4)	9.84550(10)	9.8777(4)	9.8957(4)
c/Å	10.6040(4)	10.30690(10)	10.3215(5)	10.3014(4)
α/°	63.185(4)	62.8630(10)	62.687(5)	62.813(4)
β/°	75.649(4)	74.5770(10)	75.031(4)	74.676(4)
γ/°	78.926(4)	79.9300(10)	80.935(4)	81.315(4)
Volume/Å^3	808.17(7)	759.454(16)	763.17(7)	763.75(6)
Z	1	1	1	1
ρ_{calc}g/cm^3	2.381	2.123	2.216	2.408
μ/mm^{-1}	4.743	10.292	14.230	10.166
F(000)	542.0	470.0	488.0	520.0
Crystal size/mm^3	0.18 × 0.16 × 0.12	0.14 × 0.13 × 0.1	0.16 × 0.15 × 0.1	0.12 × 0.1 × 0.08
Radiation	Mo Kα (λ = 0.71073)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.794 to 51.996	9.868 to 124.946	9.87 to 140.832	5.864 to 51.994
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -13 ≤ l ≤ 13	-9 ≤ h ≤ 10, -10 ≤ k ≤ 11, -11 ≤ l ≤ 11	-10 ≤ h ≤ 10, -12 ≤ k ≤ 10, -12 ≤ l ≤ 12	-10 ≤ h ≤ 10, -12 ≤ k ≤ 12, -12 ≤ l ≤ 12
Reflections collected	11548	7889	12792	11363
Independent reflections	3164 [R_{int} = 0.0258, R_{sigma} = 0.0232]	2337 [R_{int} = 0.0347, R_{sigma} = 0.0243]	2890 [R_{int} = 0.0499, R_{sigma} = 0.0403]	2993 [R_{int} = 0.0417, R_{sigma} = 0.0385]
Data/restraints/parameters	3164/0/189	2337/0/189	2890/0/189	2993/0/189
Goodness-of-fit on F^2	1.068	1.088	1.087	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0180, wR_2 = 0.0421	R_1 = 0.0315, wR_2 = 0.0833	R_1 = 0.0340, wR_2 = 0.0903	R_1 = 0.0272, wR_2 = 0.0641
Final R indexes [all data]	R_1 = 0.0205, wR_2 = 0.0434	R_1 = 0.0322, wR_2 = 0.0840	R_1 = 0.0376, wR_2 = 0.0930	R_1 = 0.0326, wR_2 = 0.0672
Largest diff. peak/hole / e Å^{-3}	0.64/-0.64	0.60/-0.83	0.78/-1.14	2.42/-1.42

Table S2. Distances for (plane)$\pi_{ArF}\cdots$M, (plane)$\pi_{ArF}\cdots$S, and (plane)$\pi_{ArF}\cdots$ (plane)$_{MS4}$ and (plane)$\pi_{ArF}\cdots$ (plane)π_{ArF} contacts in the structures of (**1**–**3**)·2(FXB), Å.

contact	**1**·2(FBrB)	**1**·2(FIB)	**2**·2(FBrB)	**3**·2(FBrB)
$\pi_{ArF}\cdots$M	3.4299(11)	3.4879(11)	3.4293(15)	3.4396(18)
$\pi_{ArF}\cdots$S	3.327(3)	3.337(3)	3.319(4)	3.328(4)
$\pi_{ArF}\cdots$S	3.538(2)	3.635(2)	3.531(3)	3.539(4)
$\pi_{ArF}\cdots$ π_{ArF}	3.4710(2)	3.558(3)	3.475(3)	3.469(4)

Table S3. Halogen bonds in the structures of (**1**–**3**)·2(FXB).

contact	X···Y distance, Å	Nc[a]	C–X···Y angle, °	X···Y–Z angle, °
1·2(FBrB)				
C1S–Br1S···S1–Ni1	3.6033(11)	0.99	175.01(8)	153.25(3)
C2S–Br2S···Br2S–C2S	3.5655(6)	0.96	148.49(8)	148.49(8)
C2S–Br2S···F3S–C5S	3.2544(17)	0.98	141.56(8)	140.17(14)
1·2(FIB)				
C1S–I1S···S1–Ni1	3.5605(9)	0.94	171.75(7)	150.35(3)
C2S–I2S···I2S–C2S	3.7734(4)	0.95	146.91(7)	146.91(7)
C2S–I2S···F3S–C5S	3.2967(16)	0.96	144.07(7)	140.86(14)
2·2(FBrB)				
C1S–Br1S···S1–Pd1	3.5571(14)	0.97	174.99(11)	150.61(4)
C2S–Br2S···Br2S–C2S	3.5576(7)	0.96	149.21(11)	149.21(11)
C2S–Br2S···F3S–C5S	3.256(3)	0.98	140.89(11)	139.6(2)
3·2(FBrB)				
C1S–Br1S···S1–Pt1	3.5571(17)	0.97	174.86(16)	150.12(5)

C2S–Br2S···Br2S–C2S	3.5532(8)	0.96	148.89(13)	148.89(13)
C2S–Br2S···F3S–C5S	3.257(3)	0.98	141.26(14)	139.9(2)

[a]The Normalized contact (Nc) is defined as the ratio between the separation observed in the crystal and the sum of Bondi vdW radii of interacting atoms: Nc = d/$\sum_{vdW}$; Σ_{vdW}(Br+S) = 3.65 Å, Σ_{vdW}(Br+Br) = 3.70 Å, Σ_{vdW}(Br+F) = 3.32 Å, Σ_{vdW}(I+S) = 3.78 Å, Σ_{vdW}(I+I) = 3.96 Å, Σ_{vdW}(I+F) = 3.45 Å.

Table S3. Hydrogen bonds in the structures of (**1**–**3**)·2(FXB), Å.

contact	H···Y distance, Å	Nc[a]	C···Y distance, Å	C–H···Y angle, °
1·2(FBrB)				
C2–H2A···F4S	2.5055(17)	0.94	3.467(3)	170.90(18)
C3–H3C···F3S	2.662(2)	1.0	3.421(4)	136.29(15)
C2–H2B···Br1S	3.0153(4)	0.99	3.813(4)	140.3(2)
1·2(FIB)				
C2–H2B···F4S	2.5888(16)	0.97	3.551(3)	171.5(2)
C3–H3B···F1S	2.5902(17)	0.97	3.361(3)	137.5(2)
C2–H2A···I1S	3.1268(3)	0.98	3.943(3)	142.74(18)
2·2(FBrB)				
C2–H2A···F4S	2.485(3)	0.93	3.463(5)	169.0(3)
C3–H3C···F3S	2.629(3)	0.98	3.401(6)	135.8(2)
C2–H2B···Br1S	3.0094(5)	0.99	3.822(5)	140.2(3)
3·2(FBrB)				
C2–H2B···F4S	2.504(3)	0.94	3.460(5)	168.7(3)
C3–H3A···F3S	2.642(3)	0.99	3.399(7)	136.1(3)
C2–H2A···Br1S	3.0333(6)	0.99	3.832(6)	140.5(3)

[a]Nc = d/$\sum_{vdW}$; Σ_{vdW}(H+F) = 2.67 Å, Σ_{vdW}(H+Br) = 3.05 Å, Σ_{vdW}(H+I) = 3.32 Å.

Computational details

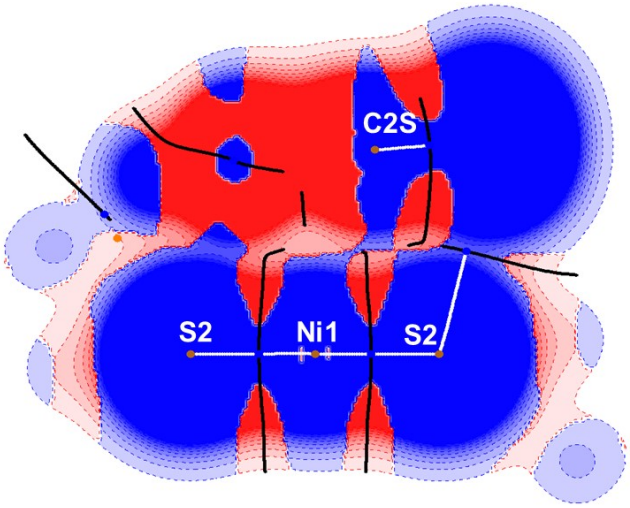

Figure S1. Projection of sign(λ_2)ρ(**r**) defined by three atoms (S2, C2S, S2) along the C2S···Ni1 bond path in **1**·(FIB).

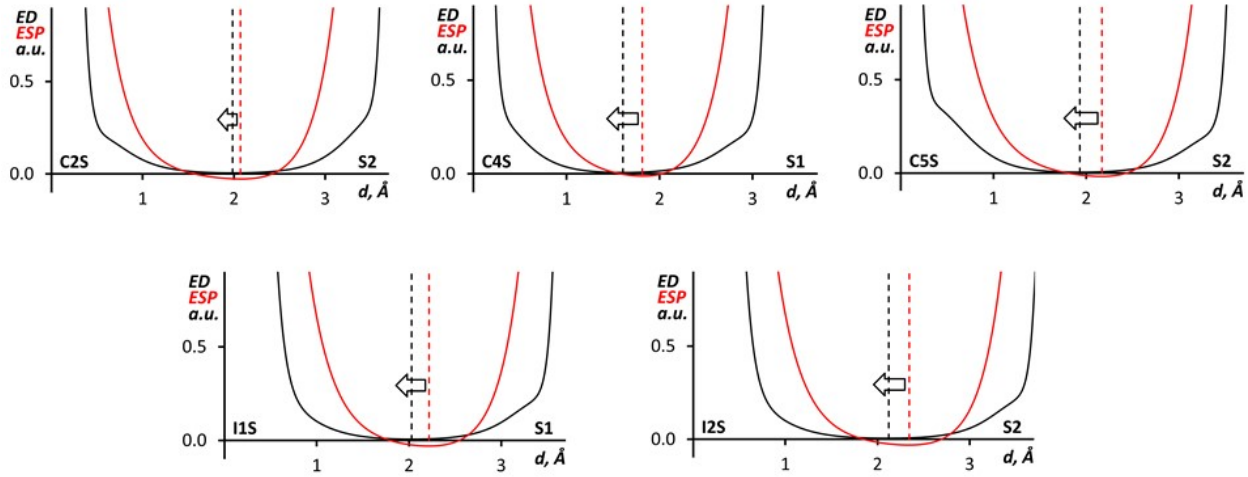

Figure S2. The ED (black) and ESP (red) 1D profiles along the C···S (*top*) and I···S (*bottom*) bond paths for **1**·(FIB).

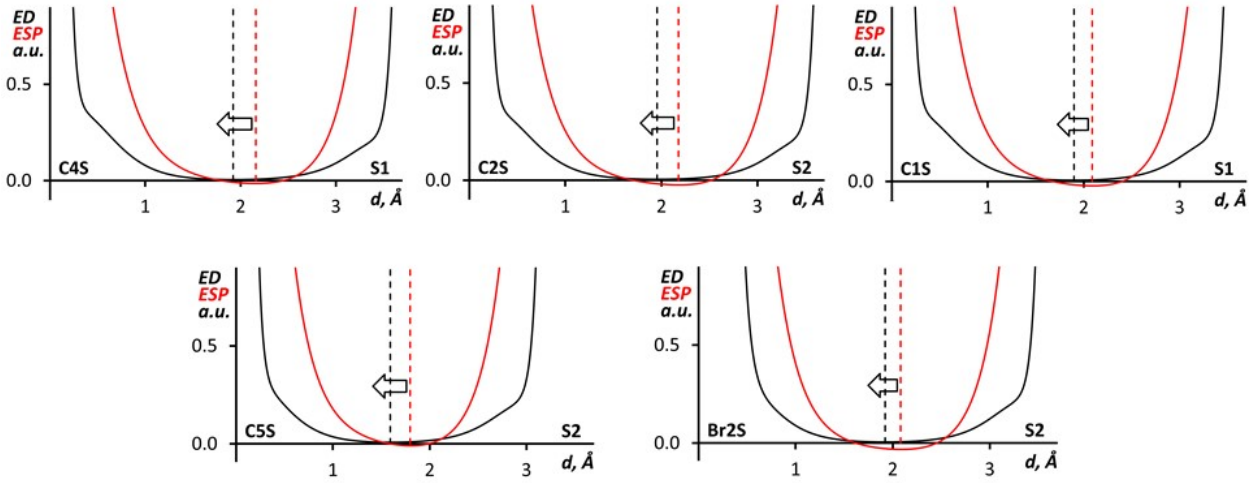

Figure S3. The ED (black) and ESP (red) 1D profiles along the C···S and Br···S bond paths for **1**·(FBrB).

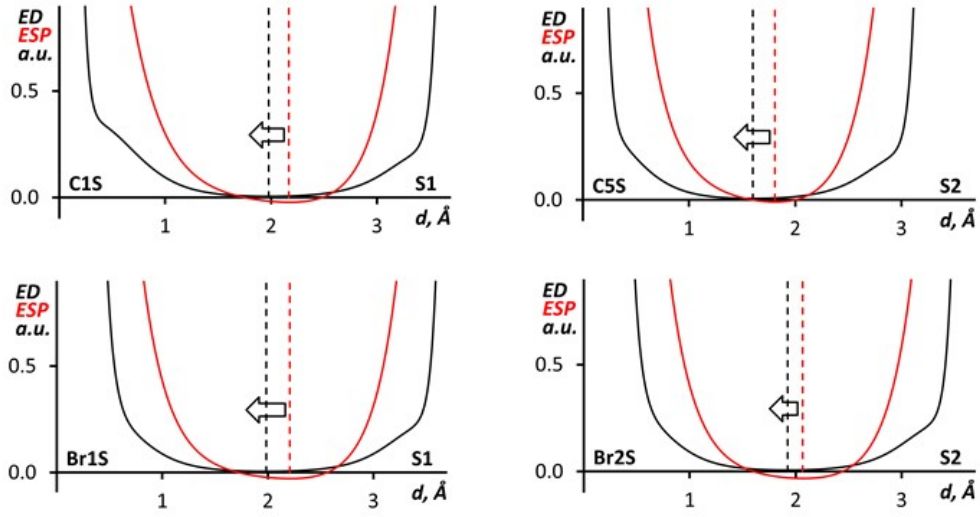

Figure S4. The ED (black) and ESP (red) 1D profiles along the C···S (*top*) and Br···S (*bottom*)bond paths for **2**·(FBrB).

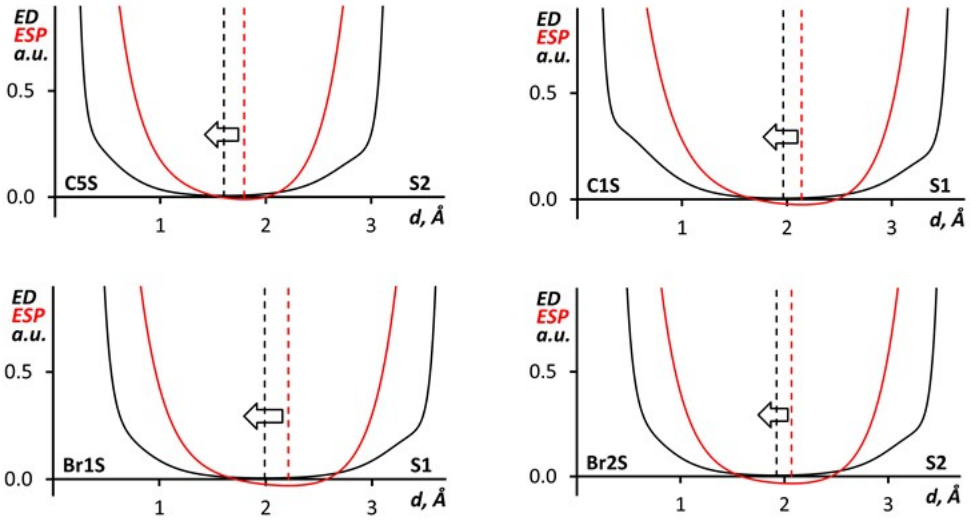

Figure S5. The ED (black) and ESP (red) 1D profiles along the C···S (*top*) and Br···S (*bottom*)bond paths for **3**·(FBrB).

Cartesian Coordinates

Dimers of Fig. 6

1·FBrB

Br	7.53830000	8.85240000	6.94100000
Br	9.63840000	6.54700000	5.57770000
F	3.82410000	5.32220000	6.30290000
F	5.50270000	3.47280000	5.23070000
F	4.75840000	7.71450000	7.07790000
F	8.10590000	4.06220000	4.88030000
C	5.61240000	6.83500000	6.53840000
C	6.95590000	7.16040000	6.37970000
C	5.12200000	5.60180000	6.14490000
C	5.97070000	4.67000000	5.59550000
C	7.80830000	6.21740000	5.81690000
C	7.30620000	4.98070000	5.43240000
Ni	8.83300000	13.98180000	8.96280000
S	6.66520000	14.11660000	9.36840000
S	8.71720000	15.97650000	9.90420000
N	6.14350000	16.48340000	10.56900000
C	7.02360000	15.66490000	10.03120000
C	7.01240000	17.58170000	12.59900000
H	7.75400000	16.97210000	12.62770000
H	6.28670000	17.22650000	13.11710000
H	7.27980000	18.42900000	12.96200000
C	4.70320000	16.16500000	10.60030000
H	4.32070000	16.48630000	11.43210000
H	4.58540000	15.20250000	10.56810000
C	6.56490000	17.76530000	11.16140000
H	5.82630000	18.39350000	11.13090000
H	7.29500000	18.13710000	10.64160000
C	3.97130000	16.80010000	9.43160000
H	4.29600000	16.42630000	8.60970000
H	4.12470000	17.74800000	9.43520000
H	3.03030000	16.62840000	9.51220000
S	11.00080000	13.84700000	8.55730000
S	8.94890000	11.98710000	8.02150000
N	11.52260000	11.48010000	7.35670000
C	10.64250000	12.29870000	7.89450000
C	10.65370000	10.38190000	5.32660000
H	9.91210000	10.99150000	5.29790000
H	11.37940000	10.73700000	4.80860000
H	10.38630000	9.53450000	4.96360000
C	12.96290000	11.79860000	7.32530000
H	13.34540000	11.47720000	6.49360000
H	13.08060000	12.76110000	7.35760000
C	11.10110000	10.19820000	6.76420000
H	11.83980000	9.57010000	6.79470000
H	10.37110000	9.82650000	7.28410000
C	13.69480000	11.16350000	8.49410000
H	13.37010000	11.53730000	9.31600000
H	13.54140000	10.21560000	8.49050000
H	14.63570000	11.33520000	8.41340000

1·FIB

Ni	6.76610000	6.99700000	4.65100000
S	6.89750000	5.01150000	3.69090000
S	8.93970000	6.84720000	4.31350000
N	9.48290000	4.51980000	3.05940000
C	9.09030000	3.24240000	2.43060000
H	8.33630000	2.86620000	2.91060000
H	9.82750000	2.61510000	2.49020000
C	10.92080000	4.84900000	3.05480000
H	11.03060000	5.81280000	3.07620000
H	11.32420000	4.51870000	2.23710000
C	8.59290000	5.32030000	3.59990000

C	11.62750000	4.23230000	4.25290000
H	12.57270000	4.39180000	4.18410000
H	11.46300000	3.28680000	4.27060000
H	11.29490000	4.63000000	5.06030000
C	8.71240000	3.44310000	0.97210000
H	9.47640000	3.75850000	0.48370000
H	8.00420000	4.08730000	0.90970000
H	8.41840000	2.60780000	0.60000000
S	6.63460000	8.98250000	5.61120000
S	4.59240000	7.14680000	4.98850000
N	4.04920000	9.47420000	6.24260000
C	4.44180000	10.75160000	6.87140000
H	5.19580000	11.12780000	6.39140000
H	3.70460000	11.37880000	6.81190000
C	2.61130000	9.14500000	6.24720000
H	2.50150000	8.18120000	6.22580000
H	2.20790000	9.47520000	7.06490000
C	4.93920000	8.67370000	5.70210000
C	1.90460000	9.76160000	5.04910000
H	0.95940000	9.60220000	5.11800000
H	2.06910000	10.70710000	5.03150000
H	2.23720000	9.36390000	4.24170000
C	4.81970000	10.55080000	8.33000000
H	4.05570000	10.23540000	8.81830000
H	5.52790000	9.90660000	8.39230000
H	5.11370000	11.38610000	8.70210000
I	5.90780000	14.51540000	8.14240000
I	8.18310000	11.98720000	6.72980000
F	11.02330000	13.32720000	6.68030000
F	10.26020000	17.58150000	8.48120000
F	11.94090000	15.72640000	7.44210000
F	7.65040000	16.99550000	8.81130000
C	8.82030000	13.87580000	7.35420000
C	7.95400000	14.82720000	7.90210000
C	10.15170000	14.20700000	7.21000000
C	8.45980000	16.06250000	8.27880000
C	10.64570000	15.43840000	7.59050000
C	9.78980000	16.37440000	8.12810000

2·FBrB

Br	7.40550000	8.93050000	6.93030000
Br	9.50350000	6.62360000	5.56870000
F	4.62520000	7.78960000	7.08830000
F	5.37190000	3.53470000	5.26000000
F	3.69310000	5.39150000	6.31940000
F	7.97250000	4.13080000	4.89430000
C	5.48550000	6.90920000	6.54520000
C	7.66170000	6.28870000	5.82280000
C	7.17970000	5.05760000	5.43660000
C	4.98760000	5.67430000	6.15710000
C	6.81760000	7.23150000	6.38210000
C	5.83810000	4.74260000	5.60680000
Pd	8.58720000	14.12490000	8.96240000
S	6.31140000	14.32120000	9.41450000
S	8.36760000	16.21920000	9.95570000
N	5.78990000	16.68410000	10.59980000
C	3.61580000	16.97670000	9.44360000
H	3.97120000	16.60490000	8.60920000
H	3.74400000	17.94790000	9.44900000
H	2.65970000	16.77340000	9.51090000
C	6.65400000	17.79070000	12.63690000
H	7.41360000	17.17160000	12.66560000
H	5.91610000	17.42790000	13.16930000
H	6.92590000	18.65760000	13.00260000
C	6.19830000	17.96940000	11.19130000
H	5.43640000	18.60120000	11.16260000
H	6.93750000	18.35650000	10.65890000
C	4.35350000	16.35840000	10.63200000
H	3.95880000	16.69710000	11.47450000
H	4.23900000	15.37520000	10.61410000
C	6.66810000	15.87340000	10.07550000

S	10.86300000	13.92860000	8.51020000
S	8.80680000	12.03060000	7.96900000
N	11.38440000	11.56570000	7.32490000
C	13.55850000	11.27310000	8.48110000
H	13.20320000	11.64490000	9.31550000
H	13.43030000	10.30190000	8.47570000
H	14.51470000	11.47640000	8.41390000
C	10.52030000	10.45920000	5.28780000
H	9.76080000	11.07820000	5.25910000
H	11.25830000	10.82190000	4.75540000
H	10.24840000	9.59220000	4.92210000
C	10.97610000	10.28040000	6.73340000
H	11.73800000	9.64860000	6.76210000
H	10.23690000	9.89330000	7.26580000
C	12.82090000	11.89140000	7.29270000
H	13.21550000	11.55280000	6.45020000
H	12.93540000	12.87460000	7.31060000
C	10.50630000	12.37640000	7.84920000

3·FBrB

Br	5.53820000	5.19250000	2.01970000
Br	3.44010000	7.50390000	3.37680000
F	9.25580000	8.72910000	2.62760000
F	8.31970000	6.33650000	1.86550000
F	4.97510000	9.99080000	4.05710000
F	7.57390000	10.58990000	3.68990000
C	5.26850000	7.82850000	3.12710000
C	7.10770000	9.37600000	3.33610000
C	7.96070000	8.45710000	2.79650000
C	6.12390000	6.89280000	2.57490000
C	7.47480000	7.20770000	2.39980000
C	5.76840000	9.07790000	3.52380000
Pt	4.36930000	0.00000000	0.00000000
S	6.64310000	-0.19860000	-0.45360000
S	4.60540000	-2.09090000	-0.99070000
N	7.19340000	-2.56080000	-1.64480000
C	6.31410000	-1.75560000	-1.11770000
C	8.61830000	-2.23860000	-1.67430000
H	8.72820000	-1.27410000	-1.66630000
H	9.00560000	-2.57520000	-2.49720000
C	6.78200000	-3.84850000	-2.23900000
H	6.06020000	-4.22890000	-1.71360000
H	7.52780000	-4.46730000	-2.21400000
C	9.36710000	-2.83860000	-0.48420000
H	10.30130000	-2.63210000	-0.55660000
H	9.24950000	-3.79160000	-0.48070000
H	9.01970000	-2.47020000	0.33150000
C	6.32080000	-3.67380000	-3.67390000
H	7.03720000	-3.30830000	-4.19740000
H	5.56940000	-3.07610000	-3.69800000
H	6.06330000	-4.52490000	-4.03390000
S	2.09560000	0.19860000	0.45360000
S	4.13330000	2.09090000	0.99070000
N	1.54530000	2.56080000	1.64480000
C	2.42460000	1.75560000	1.11770000
C	0.12040000	2.23860000	1.67430000
H	0.01050000	1.27410000	1.66630000
H	-0.26690000	2.57520000	2.49720000
C	1.95670000	3.84850000	2.23900000
H	2.67850000	4.22890000	1.71360000
H	1.21090000	4.46730000	2.21400000
C	-0.62840000	2.83860000	0.48420000
H	-1.56260000	2.63210000	0.55660000
H	-0.51080000	3.79160000	0.48070000
H	-0.28100000	2.47020000	-0.33150000
C	2.41790000	3.67380000	3.67390000
H	1.70150000	3.30830000	4.19740000
H	3.16930000	3.07610000	3.69800000
H	2.67540000	4.52490000	4.03390000

Dimers of Fig. 7 (main text)

1·FBrB

Br	7.53830000	8.85240000	6.94100000
Br	9.63840000	6.54700000	5.57770000
F	3.82410000	5.32220000	6.30290000
F	5.50270000	3.47280000	5.23070000
F	4.75840000	7.71450000	7.07790000
F	8.10590000	4.06220000	4.88030000
C	5.61240000	6.83500000	6.53840000
C	6.95590000	7.16040000	6.37970000
C	5.12200000	5.60180000	6.14490000
C	5.97070000	4.67000000	5.59550000
C	7.80830000	6.21740000	5.81690000
C	7.30620000	4.98070000	5.43240000
Ni	7.11150000	4.28800000	8.96280000
S	4.94370000	4.42280000	9.36840000
S	6.99570000	6.28260000	9.90420000
N	4.42200000	6.78960000	10.56900000
C	5.30210000	5.97110000	10.03120000
C	5.29090000	7.88780000	12.59900000
H	6.03250000	7.27820000	12.62770000
H	4.56520000	7.53270000	13.11710000
H	5.55830000	8.73520000	12.96200000
C	2.98170000	6.47120000	10.60030000
H	2.59920000	6.79250000	11.43210000
H	2.86400000	5.50860000	10.56810000
C	4.84340000	8.07150000	11.16140000
H	4.10480000	8.69960000	11.13090000
H	5.57350000	8.44320000	10.64160000
C	2.24980000	7.10630000	9.43160000
H	2.57450000	6.73250000	8.60970000
H	2.40320000	8.05410000	9.43520000
H	1.30890000	6.93450000	9.51220000
S	9.27930000	4.15320000	8.55730000
S	7.22740000	2.29330000	8.02150000
N	9.80110000	1.78630000	7.35670000
C	8.92100000	2.60490000	7.89450000
C	8.93220000	0.68810000	5.32660000
H	8.19060000	1.29770000	5.29790000
H	9.65790000	1.04320000	4.80860000
H	8.66480000	-0.15930000	4.96360000
C	11.24140000	2.10480000	7.32530000
H	11.62390000	1.78340000	6.49360000
H	11.35910000	3.06730000	7.35760000
C	9.37960000	0.50440000	6.76420000
H	10.11830000	-0.12370000	6.79470000
H	8.64960000	0.13270000	7.28410000
C	11.97330000	1.46960000	8.49410000
H	11.64860000	1.84350000	9.31600000
H	11.81990000	0.52180000	8.49050000
H	12.91420000	1.64140000	8.41340000

1·FIB

I	9.50980000	9.11260000	1.15960000
I	7.23460000	11.64080000	2.57220000
F	4.39440000	10.30070000	2.62180000
F	5.15740000	6.04640000	0.82080000
F	3.47680000	7.90150000	1.85990000
F	7.76730000	6.63240000	0.49080000
C	6.59740000	9.75220000	1.94780000
C	7.46370000	8.80080000	1.40000000
C	5.26600000	9.42090000	2.09200000
C	6.95790000	7.56540000	1.02320000
C	4.77200000	8.18960000	1.71160000
C	5.62790000	7.25360000	1.17390000
Ni	6.76610000	6.99700000	4.65100000
S	6.89750000	5.01150000	3.69090000
S	8.93970000	6.84720000	4.31350000
N	9.48290000	4.51980000	3.05940000
C	9.09030000	3.24240000	2.43060000
H	8.33630000	2.86620000	2.91060000

H	9.82750000	2.61510000	2.49020000
C	10.92080000	4.84900000	3.05480000
H	11.03060000	5.81280000	3.07620000
H	11.32420000	4.51870000	2.23710000
C	8.59290000	5.32030000	3.59990000
C	11.62750000	4.23230000	4.25290000
H	12.57270000	4.39180000	4.18410000
H	11.46300000	3.28680000	4.27060000
H	11.29490000	4.63000000	5.06030000
C	8.71240000	3.44310000	0.97210000
H	9.47640000	3.75850000	0.48370000
H	8.00420000	4.08730000	0.90970000
H	8.41840000	2.60780000	0.60000000
S	6.63460000	8.98250000	5.61120000
S	4.59240000	7.14680000	4.98850000
N	4.04920000	9.47420000	6.24260000
C	4.44180000	10.75160000	6.87140000
H	5.19580000	11.12780000	6.39140000
H	3.70460000	11.37880000	6.81190000
C	2.61130000	9.14500000	6.24720000
H	2.50150000	8.18120000	6.22580000
H	2.20790000	9.47520000	7.06490000
C	4.93920000	8.67370000	5.70210000
C	1.90460000	9.76160000	5.04910000
H	0.95940000	9.60220000	5.11800000
H	2.06910000	10.70710000	5.03150000
H	2.23720000	9.36390000	4.24170000
C	4.81970000	10.55080000	8.33000000
H	4.05570000	10.23540000	8.81830000
H	5.52790000	9.90660000	8.39230000
H	5.11370000	11.38610000	8.70210000

2·FBrB

Br	7.40550000	8.93050000	6.93030000
Br	9.50350000	6.62360000	5.56870000
F	4.62520000	7.78960000	7.08830000
F	5.37190000	3.53470000	5.26000000
F	3.69310000	5.39150000	6.31940000
F	7.97250000	4.13080000	4.89430000
C	5.48550000	6.90920000	6.54520000
C	7.66170000	6.28870000	5.82280000
C	7.17970000	5.05760000	5.43660000
C	4.98760000	5.67430000	6.15710000
C	6.81760000	7.23150000	6.38210000
C	5.83810000	4.74260000	5.60680000
Pd	7.03090000	4.37060000	8.96240000
S	4.75510000	4.56690000	9.41450000
S	6.81130000	6.46490000	9.95570000
N	4.23360000	6.92970000	10.59980000
C	2.05950000	7.22240000	9.44360000
H	2.41490000	6.85060000	8.60920000
H	2.18770000	8.19360000	9.44900000
H	1.10340000	7.01910000	9.51090000
C	5.09770000	8.03630000	12.63690000
H	5.85730000	7.41730000	12.66560000
H	4.35980000	7.67360000	13.16930000
H	5.36960000	8.90330000	13.00260000
C	4.64200000	8.21510000	11.19130000
H	3.88010000	8.84680000	11.16260000
H	5.38120000	8.60220000	10.65890000
C	2.79720000	6.60410000	10.63200000
H	2.40250000	6.94270000	11.47450000
H	2.68270000	5.62090000	10.61410000
C	5.11180000	6.11900000	10.07550000
S	9.30670000	4.17430000	8.51020000
S	7.25050000	2.27630000	7.96900000
N	9.82820000	1.81140000	7.32490000
C	12.00230000	1.51880000	8.48110000
H	11.64690000	1.89060000	9.31550000

H	11.87410000	0.54760000	8.47570000
H	12.95840000	1.72210000	8.41390000
C	8.96410000	0.70480000	5.28780000
H	8.20450000	1.32390000	5.25910000
H	9.70200000	1.06750000	4.75540000
H	8.69220000	-0.16210000	4.92210000
C	9.41980000	0.52610000	6.73340000
H	10.18170000	-0.10570000	6.76210000
H	8.68060000	0.13900000	7.26580000
C	11.26460000	2.13710000	7.29270000
H	11.65930000	1.79840000	6.45020000
H	11.37910000	3.12030000	7.31060000
C	8.95000000	2.62210000	7.84920000

3·FBrB

Br	5.53820000	5.19250000	2.01970000
Br	3.44010000	7.50390000	3.37680000
F	9.25580000	8.72910000	2.62760000
F	8.31970000	6.33650000	1.86550000
F	4.97510000	9.99080000	4.05710000
F	7.57390000	10.58990000	3.68990000
C	5.26850000	7.82850000	3.12710000
C	7.10770000	9.37600000	3.33610000
C	7.96070000	8.45710000	2.79650000
C	6.12390000	6.89280000	2.57490000
C	7.47480000	7.20770000	2.39980000
C	5.76840000	9.07790000	3.52380000
Pt	5.86360000	9.78220000	0.00000000
S	8.13740000	9.58360000	-0.45360000
S	6.09970000	7.69130000	-0.99070000
N	8.68770000	7.22140000	-1.64480000
C	7.80830000	8.02660000	-1.11770000
C	10.11260000	7.54360000	-1.67430000
H	10.22240000	8.50810000	-1.66630000
H	10.49990000	7.20700000	-2.49720000
C	8.27630000	5.93370000	-2.23900000
H	7.55450000	5.55340000	-1.71360000
H	9.02210000	5.31490000	-2.21400000
C	10.86140000	6.94370000	-0.48420000
H	11.79560000	7.15010000	-0.55660000
H	10.74370000	5.99070000	-0.48070000
H	10.51400000	7.31200000	0.33150000
C	7.81510000	6.10840000	-3.67390000
H	8.53150000	6.47400000	-4.19740000
H	7.06360000	6.70610000	-3.69800000
H	7.55750000	5.25730000	-4.03390000
S	3.58980000	9.98080000	0.45360000
S	5.62760000	11.87310000	0.99070000
N	3.03960000	12.34300000	1.64480000
C	3.91890000	11.53790000	1.11770000
C	1.61470000	12.02090000	1.67430000
H	1.50480000	11.05630000	1.66630000
H	1.22740000	12.35750000	2.49720000
C	3.45090000	13.63080000	2.23900000
H	4.17270000	14.01110000	1.71360000
H	2.70520000	14.24950000	2.21400000
C	0.86580000	12.62080000	0.48420000
H	-0.06830000	12.41440000	0.55660000
H	0.98350000	13.57380000	0.48070000
H	1.21320000	12.25240000	-0.33150000
C	3.91220000	13.45610000	3.67390000
H	3.19570000	13.09050000	4.19740000
H	4.66360000	12.85840000	3.69800000
H	4.16970000	14.30710000	4.03390000

TRIMERS

1·2(FBrB)

Ni	4.370500000	0.000000000	0.000000000
S	2.202700000	0.134800000	0.405600000

S	4.254700000	1.994700000	0.941400000
N	1.681000000	2.501700000	1.606100000
C	2.561000000	1.683100000	1.068400000
C	2.549900000	3.599900000	3.636200000
H	3.291500000	2.990300000	3.664900000
H	1.824200000	3.244800000	4.154300000
H	2.817300000	4.447300000	3.999200000
C	0.240600000	2.183200000	1.637500000
H	-0.141800000	2.504500000	2.469300000
H	0.122900000	1.220700000	1.605200000
C	2.102400000	3.783600000	2.198600000
H	1.363700000	4.411700000	2.168100000
H	2.832400000	4.155300000	1.678700000
C	-0.491200000	2.818300000	0.468800000
H	-0.166600000	2.444500000	-0.353100000
H	-0.337800000	3.766200000	0.472300000
H	-1.432200000	2.646600000	0.549400000
S	6.538300000	-0.134800000	-0.405600000
S	4.486300000	-1.994700000	-0.941400000
N	7.060000000	-2.501700000	-1.606100000
C	6.180000000	-1.683100000	-1.068400000
C	6.191100000	-3.599900000	-3.636200000
H	5.449500000	-2.990300000	-3.664900000
H	6.916800000	-3.244800000	-4.154300000
H	5.923700000	-4.447300000	-3.999200000
C	8.500400000	-2.183200000	-1.637500000
H	8.882800000	-2.504500000	-2.469300000
H	8.618100000	-1.220700000	-1.605200000
C	6.638600000	-3.783600000	-2.198600000
H	7.377300000	-4.411700000	-2.168100000
H	5.908600000	-4.155300000	-1.678700000
C	9.232200000	-2.818300000	-0.468800000
H	8.907600000	-2.444500000	0.353100000
H	9.078800000	-3.766200000	-0.472300000
H	10.173200000	-2.646600000	-0.549400000
Br	4.797200000	4.564400000	-2.021800000
Br	6.897400000	2.259000000	-3.385100000
F	1.083000000	1.034200000	-2.659900000
F	2.761600000	-0.815200000	-3.732100000
F	2.017300000	3.426500000	-1.884900000
F	5.364900000	-0.225700000	-4.082600000
C	2.871300000	2.547000000	-2.424400000
C	4.214800000	2.872500000	-2.583100000
C	2.381000000	1.313800000	-2.817900000
C	3.229600000	0.382100000	-3.367300000
C	5.067200000	1.929400000	-3.146000000
C	4.565100000	0.692700000	-3.530500000
Br	3.943800000	-4.564400000	2.021800000
Br	1.843600000	-2.259000000	3.385100000
F	7.658000000	-1.034200000	2.659900000
F	5.979400000	0.815200000	3.732100000
F	6.723700000	-3.426500000	1.884900000
F	3.376100000	0.225700000	4.082600000
C	5.869700000	-2.547000000	2.424400000
C	4.526200000	-2.872500000	2.583100000
C	6.360000000	-1.313800000	2.817900000
C	5.511400000	-0.382100000	3.367300000
C	3.673800000	-1.929400000	3.146000000
C	4.175900000	-0.692700000	3.530500000
1·2(FIB)			
I	9.509800000	9.112600000	1.159600000
I	7.234600000	11.640800000	2.572200000
F	4.394400000	10.300700000	2.621800000
F	5.157400000	6.046400000	0.820800000
F	3.476800000	7.901500000	1.859900000
F	7.767300000	6.632400000	0.490800000
C	6.597400000	9.752200000	1.947800000
C	7.463700000	8.800800000	1.400000000
C	5.266000000	9.420900000	2.092000000
C	6.957900000	7.565400000	1.023200000
C	4.772000000	8.189600000	1.711600000

C	5.627900000	7.253600000	1.173900000
Ni	6.766100000	6.997000000	4.651000000
S	6.897500000	5.011500000	3.690900000
S	8.939700000	6.847200000	4.313500000
N	9.482900000	4.519800000	3.059400000
C	9.090300000	3.242400000	2.430600000
H	8.336300000	2.866200000	2.910600000
H	9.827500000	2.615100000	2.490200000
C	10.920800000	4.849000000	3.054800000
H	11.030600000	5.812800000	3.076200000
H	11.324200000	4.518700000	2.237100000
C	8.592900000	5.320300000	3.599900000
C	11.627500000	4.232300000	4.252900000
H	12.572700000	4.391800000	4.184100000
H	11.463000000	3.286800000	4.270600000
H	11.294900000	4.630000000	5.060300000
C	8.712400000	3.443100000	0.972100000
H	9.476400000	3.758500000	0.483700000
H	8.004200000	4.087300000	0.909700000
H	8.418400000	2.607800000	0.600000000
S	6.634600000	8.982500000	5.611200000
S	4.592400000	7.146800000	4.988500000
N	4.049200000	9.474200000	6.242600000
C	4.441800000	10.751600000	6.871400000
H	5.195800000	11.127800000	6.391400000
H	3.704600000	11.378800000	6.811900000
C	2.611300000	9.145000000	6.247200000
H	2.501500000	8.181200000	6.225800000
H	2.207900000	9.475200000	7.064900000
C	4.939200000	8.673700000	5.702100000
C	1.904600000	9.761600000	5.049100000
H	0.959400000	9.602200000	5.118000000
H	2.069100000	10.707100000	5.031500000
H	2.237200000	9.363900000	4.241700000
C	4.819700000	10.550800000	8.330000000
H	4.055700000	10.235400000	8.818300000
H	5.527900000	9.906600000	8.392300000
H	5.113700000	11.386100000	8.702100000
I	4.022300000	4.881400000	8.142400000
I	6.297500000	2.353200000	6.729800000
F	9.137700000	3.693200000	6.680300000
F	8.374700000	7.947500000	8.481200000
F	10.055300000	6.092400000	7.442100000
F	5.764800000	7.361500000	8.811300000
C	6.934700000	4.241800000	7.354200000
C	6.068400000	5.193200000	7.902100000
C	8.266100000	4.573000000	7.210000000
C	6.574200000	6.428500000	8.278800000
C	8.760100000	5.804400000	7.590500000
C	7.904200000	6.740400000	8.128100000

2·2(FBrB)

Pd	4.364900000	0.000000000	0.000000000
S	2.089100000	0.196300000	0.452200000
S	4.145300000	2.094300000	0.993400000
N	1.567600000	2.559200000	1.637400000
C	-0.606500000	2.851800000	0.481300000
H	-0.251100000	2.480000000	-0.353100000
H	-0.478300000	3.823000000	0.486700000
H	-1.562600000	2.648500000	0.548500000
C	2.431700000	3.665700000	3.674600000
H	3.191300000	3.046700000	3.703200000
H	1.693800000	3.303000000	4.206900000
H	2.703600000	4.532700000	4.040200000
C	1.976000000	3.844500000	2.228900000
H	1.214100000	4.476300000	2.200300000
H	2.715200000	4.231600000	1.696600000
C	0.131200000	2.233500000	1.669700000
H	-0.263500000	2.572100000	2.512100000
H	0.016700000	1.250300000	1.651800000
C	2.445800000	1.748500000	1.113100000

S	6.640700000	-0.196300000	-0.452200000
S	4.584500000	-2.094300000	-0.993400000
N	7.162200000	-2.559200000	-1.637400000
C	9.336300000	-2.851800000	-0.481300000
H	8.980900000	-2.480000000	0.353100000
H	9.208100000	-3.823000000	-0.486700000
H	10.292400000	-2.648500000	-0.548500000
C	6.298100000	-3.665700000	-3.674600000
H	5.538500000	-3.046700000	-3.703200000
H	7.036000000	-3.303000000	-4.206900000
H	6.026200000	-4.532700000	-4.040200000
C	6.753800000	-3.844500000	-2.228900000
H	7.515700000	-4.476300000	-2.200300000
H	6.014600000	-4.231600000	-1.696600000
C	8.598600000	-2.233500000	-1.669700000
H	8.993300000	-2.572100000	-2.512100000
H	8.713100000	-1.250300000	-1.651800000
C	6.284000000	-1.748500000	-1.113100000
Br	3.990300000	-4.560000000	2.032000000
Br	1.892300000	-2.253000000	3.393700000
F	6.770600000	-3.419000000	1.874000000
F	6.023900000	0.835900000	3.702300000
F	7.702700000	-1.020900000	2.643000000
F	3.423300000	0.239700000	4.068000000
C	5.910300000	-2.538600000	2.417100000
C	3.734100000	-1.918100000	3.139500000
C	4.216200000	-0.687000000	3.525800000
C	6.408200000	-1.303700000	2.805200000
C	4.578200000	-2.861000000	2.580300000
C	5.557700000	-0.372100000	3.355500000
Br	4.739500000	4.560000000	-2.032000000
Br	6.837500000	2.253000000	-3.393700000
F	1.959200000	3.419000000	-1.874000000
F	2.705900000	-0.835900000	-3.702300000
F	1.027100000	1.020900000	-2.643000000
F	5.306500000	-0.239700000	-4.068000000
C	2.819500000	2.538600000	-2.417100000
C	4.995700000	1.918100000	-3.139500000
C	4.513600000	0.687000000	-3.525800000
C	2.321600000	1.303700000	-2.805200000
C	4.151600000	2.861000000	-2.580300000
C	3.172100000	0.372100000	-3.355500000

3·2(FBrB)

Pt	8.586000000	14.127600000	8.934500000
S	10.859800000	13.929000000	8.480900000
S	8.822100000	12.036700000	7.943800000
N	11.410100000	11.566800000	7.289600000
C	10.530800000	12.372000000	7.816800000
C	12.835000000	11.889000000	7.260100000
H	12.944800000	12.853500000	7.268200000
H	13.222300000	11.552400000	6.437300000
C	10.998700000	10.279100000	6.695500000
H	10.276900000	9.898800000	7.220800000
H	11.744500000	9.660300000	6.720500000
C	13.583800000	11.289100000	8.450200000
H	14.518000000	11.495500000	8.377900000
H	13.466200000	10.336100000	8.453800000
H	13.236400000	11.657400000	9.265900000
C	10.537500000	10.453800000	5.260600000
H	11.253900000	10.819400000	4.737100000
H	9.786100000	11.051500000	5.236500000
H	10.280000000	9.602700000	4.900600000
S	6.312300000	14.326200000	9.388100000
S	8.350000000	16.218500000	9.925100000
N	5.762000000	16.688400000	10.579300000
C	6.641300000	15.883300000	10.052200000
C	4.337100000	16.366300000	10.608800000
H	4.227200000	15.401700000	10.600700000
H	3.949800000	16.702900000	11.431700000
C	6.173400000	17.976200000	11.173400000

H	6.895100000	18.356500000	10.648100000
H	5.427600000	18.594900000	11.148400000
C	3.588300000	16.966200000	9.418700000
H	2.654100000	16.759800000	9.491100000
H	3.705900000	17.919200000	9.415100000
H	3.935700000	16.597800000	8.603000000
C	6.634600000	17.801500000	12.608300000
H	5.918200000	17.435900000	13.131900000
H	7.386000000	17.203800000	12.632400000
H	6.892100000	18.652500000	12.968400000
Br	8.260700000	9.537900000	10.954200000
Br	6.162500000	11.849300000	12.311200000
F	11.978200000	13.074500000	11.562100000
F	11.042100000	10.681900000	10.800000000
F	7.697500000	14.336200000	12.991600000
F	10.296300000	14.935300000	12.624400000
C	7.990900000	12.173900000	12.061500000
C	9.830100000	13.721400000	12.270600000
C	10.683100000	12.802500000	11.731000000
C	8.846300000	11.238200000	11.509400000
C	10.197200000	11.553100000	11.334300000
C	8.490800000	13.423300000	12.458200000
Br	8.911400000	18.717400000	6.914700000
Br	11.009500000	16.406000000	5.557700000
F	5.193900000	15.180800000	6.306800000
F	6.130000000	17.573400000	7.069000000
F	9.474600000	13.919100000	4.877300000
F	6.875800000	13.320000000	5.244500000
C	9.181100000	16.081400000	5.807400000
C	7.342000000	14.533900000	5.598300000
C	6.489000000	15.452700000	6.138000000
C	8.325800000	17.017100000	6.359600000
C	6.974900000	16.702200000	6.534700000
C	8.681300000	14.832000000	5.410700000