

Two compounds of 1-((4-bromothiophen -2-yl)methylene)-2-(perfluorophenyl)hydrazine, and 1-((4-bromo-5-methylthiophen-2-yl)methylene)-2-(perfluorophenyl)hydrazine and they crystal, molecular and electronic properties

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SUPPLEMENTARY MATERIAL FOR (I)

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Table S1 - Crystal Data and Details of the Structure Determination for (I)

Crystal Data

Formula	C11 H4 Br F5 N2 S
Formula Weight	371.13
Crystal System	monoclinic
Space group	$P2_1/n$ (No. 14)
a, b, c [Angstrom]	7.1125(1) 25.0194(5) 7.1935(2)
alpha, beta, gamma [deg]	90 109.457(2) 90
V [Ang ³]	1206.98(5)
Z	4
D(calc) [g/cm ³]	2.042
μ (CuK α) [mm ⁻¹]	6.826
F(000)	720
Crystal Size [mm]	0.09 x 0.22 x 0.59

Data Collection

Temperature (K)	298
Radiation [Angström]	CuK α 1.54178

Theta Min-Max [Degs.] 3.5, 71.7
 Dataset -8: 8 ; -30: 29 ; 0: 8
 Tot., Uniq. Data, R(int) 32397, 2331, 0.040
 Observed Data [$I > 2\sigma(I)$] 2309

Refinement

$N_{\text{ref}}, N_{\text{par}}$ 2331, 184
 R, wR^2, S 0.0296, 0.0869, 1.04
 $w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.614P]$ WHERE $P = (F_o^2 + 2F_c^2)/3$
 Max. and Av. Shift/Error 0.00, 0.00
 Min. and Max. Resd. Dens. [e/Ang^3] -0.83, 0.52

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for (I)

Atom	x	y	z	U_{eq} [Ang^2]
----	---	---	---	-----
Br1	0.88720(3)	0.03278(2)	0.19517(3)	0.0369(1)
S1	0.37921(7)	0.13328(2)	0.17957(7)	0.0308(2)
F1	0.48716(17)	0.40395(5)	0.29040(19)	0.0361(4)
F2	0.1730(2)	0.47027(4)	0.1545(2)	0.0393(4)
F3	-0.20524(19)	0.43234(5)	0.0852(2)	0.0421(4)
F4	-0.25992(18)	0.32823(5)	0.1613(2)	0.0382(4)
F5	0.05199(19)	0.26356(5)	0.31843(19)	0.0359(4)
N1	0.4476(3)	0.29908(7)	0.3804(3)	0.0315(5)
N2	0.4349(3)	0.24776(6)	0.3057(2)	0.0292(5)
C1	0.2808(3)	0.33169(8)	0.3044(3)	0.0284(5)
C2	0.3026(3)	0.38494(8)	0.2623(3)	0.0306(6)
C3	0.1428(3)	0.41910(8)	0.1921(3)	0.0315(6)
C4	-0.0481(3)	0.40018(9)	0.1568(3)	0.0329(6)
C5	-0.0741(3)	0.34721(9)	0.1970(3)	0.0317(6)
C6	0.0863(3)	0.31396(8)	0.2730(3)	0.0293(6)
C7	0.6007(3)	0.22366(8)	0.3364(3)	0.0291(6)
C8	0.6001(3)	0.16866(8)	0.2718(3)	0.0290(6)
C9	0.5025(3)	0.07690(8)	0.1473(3)	0.0333(6)
C10	0.7018(3)	0.08556(8)	0.2060(3)	0.0313(6)
C11	0.7608(3)	0.13792(8)	0.2779(3)	0.0301(6)

$U_{\text{eq}} = 1/3$ of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters

Atom	x	y	z	U_{iso} [Ang^2]
----	---	---	---	-----
H1	0.563(4)	0.3152(10)	0.413(4)	0.0380
H7	0.72309	0.24150	0.40075	0.0350
H9	0.43956	0.04409	0.09539	0.0400
H11	0.89501	0.15004	0.32432	0.0360

=====
 The Temperature Factor has the Form of Exp(-T) Where

$$T = 8(\pi^2)U(\text{Sin}(\text{Theta})/\text{Lambda})^2 \text{ for Isotropic Atoms}$$

Table S4 - Anisotropic Displacement Parameters for (I)

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Br1	0.0393(2)	0.0294(2)	0.0400(2)	-0.0005(1)	0.0106(1)	0.0079(1)
S1	0.0289(3)	0.0283(3)	0.0331(3)	-0.0004(2)	0.0077(2)	0.0000(2)
F1	0.0327(6)	0.0285(6)	0.0485(7)	-0.0013(5)	0.0154(5)	-0.0030(5)
F2	0.0471(8)	0.0245(6)	0.0476(8)	0.0053(5)	0.0174(6)	0.0027(5)
F3	0.0380(7)	0.0374(7)	0.0495(8)	0.0057(6)	0.0129(6)	0.0120(5)
F4	0.0290(6)	0.0397(7)	0.0462(7)	-0.0016(5)	0.0130(5)	-0.0007(5)
F5	0.0350(6)	0.0281(6)	0.0466(7)	0.0025(5)	0.0161(5)	-0.0018(5)
N1	0.0301(8)	0.0253(8)	0.0363(9)	-0.0030(7)	0.0074(7)	-0.0011(7)
N2	0.0334(8)	0.0241(8)	0.0299(8)	0.0007(6)	0.0102(7)	0.0009(6)
C1	0.0315(10)	0.0262(9)	0.0275(9)	-0.0023(7)	0.0097(7)	0.0022(7)
C2	0.0312(10)	0.0305(10)	0.0312(10)	-0.0035(8)	0.0117(8)	-0.0025(8)
C3	0.0394(11)	0.0238(9)	0.0327(10)	0.0005(8)	0.0138(8)	0.0010(8)
C4	0.0333(10)	0.0319(10)	0.0328(10)	0.0006(8)	0.0100(8)	0.0075(8)
C5	0.0298(9)	0.0346(11)	0.0320(10)	-0.0038(8)	0.0122(8)	0.0003(8)
C6	0.0363(11)	0.0240(10)	0.0285(9)	-0.0008(7)	0.0119(8)	0.0002(8)
C7	0.0312(10)	0.0264(10)	0.0281(9)	0.0006(7)	0.0078(7)	-0.0007(7)
C8	0.0314(10)	0.0270(10)	0.0273(9)	0.0024(7)	0.0080(7)	0.0000(7)
C9	0.0374(10)	0.0268(10)	0.0337(10)	-0.0002(8)	0.0093(8)	0.0000(8)
C10	0.0348(10)	0.0278(10)	0.0297(10)	0.0019(7)	0.0088(8)	0.0047(8)
C11	0.0323(10)	0.0293(10)	0.0281(10)	0.0016(7)	0.0093(8)	0.0006(8)

=====
 The Temperature Factor has the Form of Exp(-T) Where

$$T = 8(\pi^2)U(\text{Sin}(\text{Theta})/\text{Lambda})^2 \text{ for Isotropic Atoms}$$

$T = 2(\pi^2)\text{Sum}_{ij}(h(i)h(j)U(i,j)A^*(i)A^*(j))$, for Anisotropic Atoms. $A^*(i)$ are Reciprocal Axial Lengths and $h(i)$ are the Reflection Indices.

Table S5 - Bond Distances (Angström) for (I)

Br1	-C10	1.886(2)	N1	-H1	0.87(3)
S1	-C8	1.731(2)	C2	-C3	1.377(3)
S1	-C9	1.717(2)	C3	-C4	1.379(3)
F1	-C2	1.347(3)	C4	-C5	1.382(3)
F2	-C3	1.341(2)	C5	-C6	1.370(3)
F3	-C4	1.334(3)	C7	-C8	1.452(3)
F4	-C5	1.346(3)	C8	-C11	1.366(3)
F5	-C6	1.345(2)	C9	-C10	1.355(3)
N1	-N2	1.383(2)	C10	-C11	1.420(3)
N1	-C1	1.393(3)	C7	-H7	0.9500

N2	-C7	1.277(3)	C9	-H9	0.9500
C1	-C2	1.386(3)	C11	-H11	0.9500
C1	-C6	1.398(3)			

Table S6 - Bond Angles (Degs.) for (I)

C8	-S1	-C9	91.88(10)	F4	-C5	-C4	119.32(19)
N2	-N1	-C1	117.03(19)	F5	-C6	-C5	118.2(2)
N1	-N2	-C7	115.74(19)	F5	-C6	-C1	120.54(19)
N1	-C1	-C2	120.4(2)	C1	-C6	-C5	121.31(19)
N1	-C1	-C6	123.05(19)	N2	-C7	-C8	119.23(19)
C2	-C1	-C6	116.51(19)	S1	-C8	-C7	120.85(17)
C1	-N1	-H1	115.9(17)	C7	-C8	-C11	127.6(2)
N2	-N1	-H1	117.8(17)	S1	-C8	-C11	111.54(15)
F1	-C2	-C3	118.70(18)	S1	-C9	-C10	110.79(15)
F1	-C2	-C1	118.75(19)	Br1	-C10	-C9	123.26(16)
C1	-C2	-C3	122.6(2)	Br1	-C10	-C11	122.36(17)
F2	-C3	-C4	120.31(19)	C9	-C10	-C11	114.38(19)
C2	-C3	-C4	119.76(19)	C8	-C11	-C10	111.4(2)
F2	-C3	-C2	119.9(2)	N2	-C7	-H7	120.00
C3	-C4	-C5	118.9(2)	C8	-C7	-H7	120.00
F3	-C4	-C3	120.73(19)	S1	-C9	-H9	125.00
F3	-C4	-C5	120.4(2)	C10	-C9	-H9	125.00
C4	-C5	-C6	120.9(2)	C8	-C11	-H11	124.00
F4	-C5	-C6	119.74(19)	C10	-C11	-H11	124.00

Table S7 - Torsion Angles (Degs.) for (I)

C9	-S1	-C8	-C11	-0.35(17)
C9	-S1	-C8	-C7	-178.76(18)
C8	-S1	-C9	-C10	0.33(17)
N2	-N1	-C1	-C6	43.9(3)
N2	-N1	-C1	-C2	-138.4(2)
C1	-N1	-N2	-C7	162.27(19)
N1	-N2	-C7	-C8	176.83(18)
N1	-C1	-C2	-C3	-178.2(2)
N1	-C1	-C6	-F5	0.8(3)
C6	-C1	-C2	-C3	-0.4(3)
C2	-C1	-C6	-C5	2.6(3)
C6	-C1	-C2	-F1	179.92(16)
C2	-C1	-C6	-F5	-176.94(18)
N1	-C1	-C6	-C5	-179.7(2)
N1	-C1	-C2	-F1	2.1(3)
F1	-C2	-C3	-F2	-0.5(3)
C1	-C2	-C3	-C4	-1.6(3)
F1	-C2	-C3	-C4	178.15(18)
C1	-C2	-C3	-F2	179.81(19)
C2	-C3	-C4	-C5	1.3(3)
C2	-C3	-C4	-F3	-178.70(19)
F2	-C3	-C4	-C5	179.95(19)
F2	-C3	-C4	-F3	-0.1(3)
C3	-C4	-C5	-C6	0.8(3)

C3	-C4	-C5	-F4	-179.37(18)
F3	-C4	-C5	-F4	0.7(3)
F3	-C4	-C5	-C6	-179.14(19)
C4	-C5	-C6	-C1	-2.8(3)
C4	-C5	-C6	-F5	176.66(18)
F4	-C5	-C6	-F5	-3.1(3)
F4	-C5	-C6	-C1	177.36(18)
N2	-C7	-C8	-C11	174.6(2)
N2	-C7	-C8	-S1	-7.3(3)
S1	-C8	-C11	-C10	0.3(2)
C7	-C8	-C11	-C10	178.6(2)
S1	-C9	-C10	-Br1	179.47(11)
S1	-C9	-C10	-C11	-0.2(2)
Br1	-C10	-C11	-C8	-179.73(15)
C9	-C10	-C11	-C8	0.0(3)

Table S8 - Contact Distances (Angström) for (I)

Br1	.C2_e	3.612(2)	F3	.F4	2.7162(18)
Br1	.C3_e	3.657(2)	F3	.F1_k	3.1018(19)
Br1	.F1_a	3.3372(13)	F3	.F2	2.737(2)
Br1	.F2_a	3.3387(14)	F3	.Br1_m	3.4085(14)
Br1	.F3_b	3.4421(14)	F3	.Br1_l	3.4421(14)
Br1	.F3_d	3.4085(14)	F3	.F2_j	3.0375(17)
Br1	.H9_c	3.2000	F4	.F3	2.7162(18)
Br1	.H9	3.0300	F4	.F1_k	2.9666(18)
Br1	.H11	3.0700	F4	.C7_k	3.201(2)
S1	.N2	2.9907(16)	F4	.F5	2.6733(19)
S1	.C10	2.537(2)	F4	.N1_k	3.087(3)
S1	.F1_f	3.3585(14)	F5	.F4	2.6733(19)
S1	.N1_f	3.538(2)	F5	.N1	2.841(3)
S1	.C4_g	3.402(2)	F5	.N2	2.784(3)
S1	.C5_e	3.629(2)	F1	.H1	2.38(3)
S1	.C5_g	3.658(2)	F4	.H1_k	2.55(3)
S1	.H1_f	2.74(3)	F4	.H7_k	2.8000
F1	.F2	2.6919(18)	F4	.H11_m	2.8700
F1	.F3_h	3.1018(19)	F5	.H7_k	2.6600
F1	.F4_h	2.9666(18)	N1	.F1	2.739(2)
F1	.N1	2.739(2)	N1	.F4_h	3.087(3)
F1	.Br1_i	3.3372(13)	N1	.F5	2.841(3)
F1	.S1_g	3.3585(14)	N1	.S1_g	3.538(2)
F2	.F3_j	3.0375(17)	N2	.F5	2.784(3)
F2	.F1	2.6919(18)	N2	.S1	2.9907(16)
F2	.F3	2.737(2)	N2	.C6	2.925(3)
F2	.Br1_i	3.3387(14)	N1	.H7	2.4000
F2	.F2_j	3.0929(19)	C1	.C7_f	3.467(3)
C1	.C4	2.807(3)	C8	.C6_e	3.583(3)
C1	.C7	3.491(3)	C9	.C4_e	3.473(3)
C1	.C11_n	3.539(3)	C9	.C11	2.332(3)
N2	.H7_f	2.8100	C10	.C3_e	3.581(3)
C2	.C5	2.730(3)	C10	.C2_e	3.574(3)
C2	.C10_n	3.574(3)	C10	.C8	2.302(3)

C2	.Br1_n	3.612(2)	C11	.C1_e	3.539(3)
C2	.C8_f	3.597(3)	C11	.C2_g	3.445(3)
C2	.C11_f	3.445(3)	C11	.C9	2.332(3)
C3	.C10_n	3.581(3)	C2	.H1	2.51(3)
C3	.C6	2.752(3)	C7	.H11	2.8100
C3	.Br1_n	3.657(2)	C7	.H1	2.39(3)
C4	.C9_n	3.473(3)	C11	.H7	2.7800
C4	.C1	2.807(3)	H1	.F1	2.38(3)
C4	.S1_f	3.402(2)	H1	.F4_h	2.55(3)
C5	.S1_n	3.629(2)	H1	.C2	2.51(3)
C5	.C2	2.730(3)	H1	.C7	2.39(3)
C5	.S1_f	3.658(2)	H1	.H7	2.1800
C6	.C3	2.752(3)	H1	.S1_g	2.74(3)
C6	.N2	2.925(3)	H7	.F4_h	2.8000
C6	.C7_f	3.313(3)	H7	.F5_h	2.6600
C6	.C8_n	3.583(3)	H7	.N1	2.4000
C7	.C1_g	3.467(3)	H7	.C11	2.7800
C7	.F4_h	3.201(2)	H7	.H1	2.1800
C7	.C1	3.491(3)	H7	.N2_g	2.8100
C7	.C6_g	3.313(3)	H9	.Br1	3.0300
C8	.C10	2.302(3)	H9	.Br1_c	3.2000
C8	.C2_g	3.597(3)	H11	.Br1	3.0700
H11	.C7	2.8100	H11	.F4_d	2.8700

Table S9 - Hydrogen Bonds (Angström, Degs.) for (I)

P2₁/n R = 0.03

N1	-- H1	.. F1	0.87(3)	2.38(3)	2.739(2)	105(2)	.
N1	-- H1	.. F4	0.87(3)	2.55(3)	3.087(3)	121(2)	1_655
N1	-- H1	.. S1	0.87(3)	2.74(3)	3.538(2)	152(2)	4_555

Translation of Symmetry Code to Equiv. Pos

a=[2645.00] = [2_645] = 3/2-x,-1/2+y,1/2-z
b=[2545.00] = [2_545] = 1/2-x,-1/2+y,1/2-z
c=[3655.00] = [3_655] = 1-x,-y,-z
d=[4655.00] = [4_766] = 3/2+x,1/2-y,1/2+z
e=[4554.00] = [4_665] = 1/2+x,1/2-y,-1/2+z
f=[4454.00] = [4_565] = -1/2+x,1/2-y,-1/2+z
g=[4555.00] = [4_666] = 1/2+x,1/2-y,1/2+z
h=[1655.00] = [1_655] = 1+x,y,z
i=[2655.00] = [2_655] = 3/2-x,1/2+y,1/2-z
j=[3565.00] = [3_565] = -x,1-y,-z
k=[1455.00] = [1_455] = -1+x,y,z
l=[2555.00] = [2_555] = 1/2-x,1/2+y,1/2-z
m=[4354.00] = [4_465] = -3/2+x,1/2-y,-1/2+z
n=[4455.00] = [4_566] = -1/2+x,1/2-y,1/2+z

CCDC_2027085. Crystallographic data for the structures reported in this paper will be available from the Cambridge Crystallographic Data Centre.

SUPPLEMENTARY MATERIAL FOR (II)

Table S1 - Crystal Data and Details of the Structure Determination for (II)

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: (II)

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters for (II)

Table S4 - Anisotropic Displacement Parameters for (II)

Table S5 - Bond Distances (Angström) for (II)

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Table S7 - Torsion Angles (Degs.) for (II)

Table S8 - Contact Distances (Angström) for (II)

Table S9 - Hydrogen Bonds (Angström, Degs.) for (II)

Table S1 - Crystal Data and Details of the Structure Determination for (II)

Crystal Data

Formula	C12 H6 Br F5 N2 S
Formula Weight	385.16
Crystal System	monoclinic
Space group	<i>Pn</i> (No. 7)
a, b, c [Angstrom]	7.1916(3) 13.5415(5) 7.2384(4)
alpha, beta, gamma [deg]	90 109.951(6) 90
V [Ang**3]	662.61(6)
Z	2
D(calc) [g/cm**3]	1.930
Mu(MoKa) [/mm]	3.311
F(000)	376
Crystal Size [mm]	0.06 x 0.31 x 0.59

Data Collection

Temperature (K)	298
Radiation [Angström]	MoK α 0.71073
Theta Min-Max [Degs.]	1.5, 32.8
Dataset	-10: 10 ; -20: 20 ; -10: 10
Tot., Uniq. Data, R(int)	11109, 4379, 0.051
Observed Data [I > 0.0 sigma(I)]	3840

Refinement

N _{ref} , N _{par}	4379, 194
R, wR ² , S	0.0447, 0.1097, 1.03
w = 1/[$\sigma^2(F_o^2) + (0.0540P)^2$]	WHERE P = ($F_o^2 + 2 F_c^2$)/3
Max. and Av. Shift/Error	0.00, 0.00
Flack x	0.007(7)
Min. and Max. Resd. Dens. [e/Ang ³]	-1.14, 1.06

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for (II)

Atom	x	y	z	U _{eq} [Å ²]
---	---	---	---	-----
Br1	0.19920(8)	0.38964(3)	0.01552(8)	0.0291(1)
S1	0.2039(2)	0.21311(7)	0.5228(2)	0.0209(2)
F1	0.1208(5)	-0.2899(2)	0.4434(5)	0.0285(9)
F2	0.2527(5)	-0.4096(2)	0.7594(6)	0.0320(10)
F3	0.3017(5)	-0.3383(2)	1.1247(5)	0.0339(10)
F4	0.2200(5)	-0.1460(2)	1.1700(4)	0.0288(9)
F5	0.0682(5)	-0.0276(2)	0.8559(5)	0.0273(8)
N1	0.0168(7)	-0.0965(3)	0.4711(7)	0.0235(11)
N2	0.0872(6)	-0.0014(3)	0.4789(6)	0.0216(11)
C1	0.0920(7)	-0.1547(3)	0.6386(7)	0.0197(12)
C2	0.1387(7)	-0.2529(4)	0.6209(7)	0.0222(12)
C3	0.2084(7)	-0.3155(4)	0.7819(8)	0.0240(14)
C4	0.2339(7)	-0.2794(4)	0.9680(7)	0.0247(12)
C5	0.1923(9)	-0.1808(3)	0.9894(8)	0.0220(14)
C6	0.1178(8)	-0.1208(3)	0.8268(8)	0.0204(12)
C7	0.0584(7)	0.0418(3)	0.3143(7)	0.0209(12)
C8	0.1200(7)	0.1434(4)	0.3111(7)	0.0207(12)
C9	0.2360(7)	0.3175(4)	0.3969(8)	0.0245(12)
C10	0.1840(7)	0.2957(3)	0.2017(8)	0.0220(12)
C11	0.1171(7)	0.1972(3)	0.1502(7)	0.0223(12)
C12	0.3035(9)	0.4126(4)	0.5034(9)	0.0319(16)

U_{eq} = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters for (II)

Atom	x	y	z	U _{iso} [Å ²]
---	---	---	---	-----
H1	-0.007(10)	-0.134(4)	0.375(11)	0.0280
H7	-0.00178	0.00801	0.19717	0.0250
H11	0.07636	0.17252	0.02276	0.0270
H12A	0.41397	0.40034	0.62094	0.0480
H12B	0.19728	0.44123	0.53725	0.0480
H12C	0.34255	0.45729	0.42036	0.0480

=====

The Temperature Factor has the Form of Exp(-T) Where

$T = 8(\pi^2)U(\sin(\theta)/\lambda)^2$ for Isotropic Atoms

Table S4 - Anisotropic Displacement Parameters for (II)

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
---	-----	-----	-----	-----	-----	-----
Br1	0.0330(2)	0.0268(2)	0.0250(2)	0.0101(2)	0.0067(2)	0.0041(2)
S1	0.0241(4)	0.0230(4)	0.0130(4)	-0.0003(5)	0.0030(4)	-0.0012(6)

F1	0.0451(18)	0.0245(14)	0.0174(15)	-0.0058(11)	0.0125(13)	-0.0032(12)
F2	0.0446(19)	0.0204(13)	0.0300(18)	0.0002(13)	0.0115(15)	0.0047(13)
F3	0.0443(18)	0.0313(16)	0.0190(16)	0.0080(12)	0.0017(14)	0.0033(14)
F4	0.0391(18)	0.0323(16)	0.0118(14)	-0.0036(13)	0.0046(13)	0.0009(14)
F5	0.0391(16)	0.0208(13)	0.0207(15)	-0.0023(11)	0.0086(13)	0.0023(12)
N1	0.031(2)	0.0211(18)	0.0139(19)	-0.0011(14)	0.0017(17)	-0.0016(16)
N2	0.0205(18)	0.0219(18)	0.0168(19)	0.0011(15)	-0.0010(15)	-0.0006(14)
C1	0.020(2)	0.020(2)	0.017(2)	-0.0003(16)	0.0036(16)	-0.0042(16)
C2	0.024(2)	0.029(2)	0.013(2)	-0.0046(17)	0.0057(17)	-0.0049(18)
C3	0.027(2)	0.020(2)	0.025(3)	-0.0011(18)	0.0087(19)	-0.0026(17)
C4	0.028(2)	0.028(2)	0.015(2)	0.0043(18)	0.0032(18)	0.0008(19)
C5	0.0236(19)	0.027(2)	0.017(3)	-0.0030(18)	0.009(2)	-0.002(2)
C6	0.026(2)	0.018(2)	0.016(2)	0.0001(16)	0.0055(19)	0.0005(17)
C7	0.026(2)	0.021(2)	0.014(2)	-0.0025(16)	0.0046(17)	0.0006(18)
C8	0.022(2)	0.022(2)	0.016(2)	0.0001(17)	0.0036(16)	0.0014(17)
C9	0.026(2)	0.025(2)	0.020(2)	0.0010(18)	0.0048(19)	0.0011(18)
C10	0.021(2)	0.023(2)	0.019(2)	0.0049(18)	0.0028(17)	0.0024(17)
C11	0.025(2)	0.024(2)	0.015(2)	0.0037(17)	0.0029(17)	0.0053(18)
C12	0.034(3)	0.029(2)	0.029(3)	-0.006(2)	0.006(2)	-0.006(2)

=====

The Temperature Factor has the Form of $\text{Exp}(-T)$ Where

$T = 8(\pi^2)U(\text{Sin}(\text{Theta})/\text{Lambda})^2$ for Isotropic Atoms

$T = 2(\pi^2)\text{Sum}_{ij}(h(i)h(j)U(i,j)\text{Astar}(i)\text{A}^*(j))$, for Anisotropic Atoms. $\text{A}^*(i)$ are Reciprocal Axial Lengths and $h(i)$ are the Reflection Indices.

Table S5 - Bond Distances (Angström) for (II)

Br1	-C10	1.883(5)	C2	-C3	1.389(7)
S1	-C8	1.724(5)	C3	-C4	1.385(7)
S1	-C9	1.739(6)	C4	-C5	1.389(7)
F1	-C2	1.344(6)	C5	-C6	1.379(7)
F2	-C3	1.337(6)	C7	-C8	1.448(7)
F3	-C4	1.335(6)	C8	-C11	1.368(7)
F4	-C5	1.339(6)	C9	-C12	1.494(8)
F5	-C6	1.348(5)	C9	-C10	1.365(8)
N1	-N2	1.378(6)	C10	-C11	1.424(6)
N1	-C1	1.391(6)	C7	-H7	0.9300
N2	-C7	1.279(6)	C11	-H11	0.9300
C1	-C2	1.388(7)	C12	-H12A	0.9600
C1	-C6	1.389(7)	C12	-H12B	0.9600
N1	-H1	0.83(7)	C12	-H12C	0.9600

Table S6 - Bond Angles (Degs.) for (II)

C8	-S1	-C9	92.8(3)	F5	-C6	-C1	120.6(4)
N2	-N1	-C1	117.8(4)	N2	-C7	-C8	119.8(4)
N1	-N2	-C7	116.7(4)	C7	-C8	-C11	127.1(4)
N1	-C1	-C2	119.8(4)	S1	-C8	-C7	121.5(4)
N1	-C1	-C6	123.3(4)	S1	-C8	-C11	111.4(4)
C2	-C1	-C6	116.9(4)	C10	-C9	-C12	130.3(5)

N2	-N1	-H1	125(5)	S1	-C9	-C10	109.2(4)
C1	-N1	-H1	107(5)	S1	-C9	-C12	120.5(4)
F1	-C2	-C1	119.9(4)	Br1	-C10	-C9	122.2(4)
F1	-C2	-C3	117.7(5)	Br1	-C10	-C11	122.8(4)
C1	-C2	-C3	122.5(5)	C9	-C10	-C11	115.0(4)
F2	-C3	-C2	120.8(5)	C8	-C11	-C10	111.7(4)
C2	-C3	-C4	119.4(5)	N2	-C7	-H7	120.00
F2	-C3	-C4	119.8(5)	C8	-C7	-H7	120.00
F3	-C4	-C5	120.7(4)	C8	-C11	-H11	124.00
F3	-C4	-C3	120.3(5)	C10	-C11	-H11	124.00
C3	-C4	-C5	119.1(5)	C9	-C12	-H12A	109.00
F4	-C5	-C6	120.7(4)	C9	-C12	-H12B	109.00
F4	-C5	-C4	118.8(4)	C9	-C12	-H12C	109.00
C4	-C5	-C6	120.5(5)	H12A	-C12	-H12B	109.00
C1	-C6	-C5	121.7(4)	H12A	-C12	-H12C	109.00
F5	-C6	-C5	117.7(5)	H12B	-C12	-H12C	109.00

Table S7 - Torsion Angles (Degrees) for (II)

C9	-S1	-C8	-C11	0.3(4)
C9	-S1	-C8	-C7	-178.4(5)
C8	-S1	-C9	-C10	-0.5(4)
C8	-S1	-C9	-C12	177.4(5)
N2	-N1	-C1	-C6	44.3(8)
N2	-N1	-C1	-C2	-138.0(5)
C1	-N1	-N2	-C7	162.2(5)
N1	-N2	-C7	-C8	177.1(5)
N1	-C1	-C6	-F5	0.5(9)
C6	-C1	-C2	-C3	-0.1(8)
C2	-C1	-C6	-C5	2.0(8)
C6	-C1	-C2	-F1	-178.7(5)
N1	-C1	-C2	-C3	-178.0(5)
N1	-C1	-C6	-C5	179.8(6)
C2	-C1	-C6	-F5	-177.2(5)
N1	-C1	-C2	-F1	3.4(8)
F1	-C2	-C3	-F2	-1.1(8)
C1	-C2	-C3	-C4	-0.3(8)
C1	-C2	-C3	-F2	-179.7(5)
F1	-C2	-C3	-C4	178.3(5)
C2	-C3	-C4	-F3	-179.7(5)
C2	-C3	-C4	-C5	-1.1(8)
F2	-C3	-C4	-F3	-0.3(8)
F2	-C3	-C4	-C5	178.3(5)
C3	-C4	-C5	-C6	3.0(9)
F3	-C4	-C5	-C6	-178.4(5)
C3	-C4	-C5	-F4	-179.0(5)
F3	-C4	-C5	-F4	-0.5(9)
C4	-C5	-C6	-C1	-3.6(9)
F4	-C5	-C6	-F5	-2.2(9)
C4	-C5	-C6	-F5	175.7(5)
F4	-C5	-C6	-C1	178.6(5)
N2	-C7	-C8	-C11	173.5(5)

N2	-C7	-C8	-S1	-8.1(7)
C7	-C8	-C11	-C10	178.5(5)
S1	-C8	-C11	-C10	0.0(6)
S1	-C9	-C10	-Br1	-179.7(3)
S1	-C9	-C10	-C11	0.5(6)
C12	-C9	-C10	-Br1	2.7(9)
C12	-C9	-C10	-C11	-177.1(6)
Br1	-C10	-C11	-C8	179.9(4)
C9	-C10	-C11	-C8	-0.4(7)

Table S8 - Contact Distances (Angström) for (II)

Br1	.F2_a	3.386(3)	F3	.F4	2.714(4)
Br1	.C12	3.365(6)	F3	.F1_k	3.081(5)
Br1	.F3_c	3.338(4)	F3	.Br1_l	3.338(4)
Br1	.C2_b	3.515(5)	F4	.N1_k	3.084(6)
Br1	.F1_b	3.517(4)	F4	.C7_k	3.121(5)
Br1	.C3_b	3.649(5)	F4	.F5	2.690(4)
Br1	.H11	3.0800	F4	.F1_k	3.031(4)
Br1	.H12C	2.9000	F4	.F3	2.714(4)
Br1	.H12C_d	3.1800	F5	.N2	2.801(5)
S1	.N2	3.010(4)	F5	.F4	2.690(4)
S1	.C10	2.539(5)	F5	.N1	2.840(6)
S1	.C4_e	3.387(6)	F1	.H1	2.29(6)
S1	.C5_e	3.630(7)	F1	.H12A_e	2.7400
S1	.C3_e	3.663(6)	F2	.H12B_j	2.5300
S1	.C5_b	3.629(7)	F4	.H1_k	2.56(8)
S1	.H12A	2.9100	F4	.H7_k	2.6700
S1	.H12B	3.0900	F5	.H7_k	2.7300
S1	.H1_f	2.89(7)	N1	.F1	2.750(5)
F1	.F2	2.698(5)	N1	.F4_g	3.084(6)
F1	.F3_g	3.081(5)	N1	.F5	2.840(6)
F1	.F4_g	3.031(4)	N2	.C6	2.937(7)
F1	.N1	2.750(5)	N2	.S1	3.010(4)
F1	.Br1_h	3.517(4)	N2	.F5	2.801(5)
F2	.Br1_i	3.386(3)	N1	.H7	2.4000
F2	.F3	2.723(5)	C1	.C7_f	3.506(7)
F2	.C12_j	3.135(7)	C1	.C4	2.814(7)
F2	.F1	2.698(5)	C1	.C7	3.502(6)
F3	.F2	2.723(5)	C1	.C8_f	3.573(7)
C1	.C11_h	3.493(7)	C8	.C6_b	3.556(8)
N2	.H7_f	2.8400	C8	.C1_e	3.573(7)
C2	.C5	2.741(7)	C9	.C3_e	3.597(8)
C2	.C10_h	3.560(8)	C9	.C4_b	3.478(8)
C2	.Br1_h	3.515(5)	C9	.C11	2.352(7)
C2	.C8_f	3.581(7)	C10	.C2_b	3.560(8)
C2	.C11_f	3.457(7)	C10	.C8	2.311(7)
C3	.S1_f	3.663(6)	C11	.C6_b	3.540(8)
C3	.C6	2.762(7)	C11	.C1_b	3.493(7)
C3	.Br1_h	3.649(5)	C11	.C2_e	3.457(7)
C3	.C9_f	3.597(8)	C11	.C9	2.352(7)
C4	.S1_f	3.387(6)	C12	.Br1	3.365(6)

C4	.C1	2.814(7)	C12	.F2_m	3.135(7)
C4	.C9_h	3.478(8)	C2	.H1	2.36(7)
C5	.S1_f	3.630(7)	C6	.H1	3.09(8)
C5	.C2	2.741(7)	C7	.H11	2.7900
C5	.S1_h	3.629(7)	C7	.H1	2.50(6)
C6	.N2	2.937(7)	C10	.H12C	2.7100
C6	.C7_f	3.375(8)	C11	.H7	2.7600
C6	.C3	2.762(7)	H1	.F1	2.29(6)
C6	.C11_h	3.540(8)	H1	.F4_g	2.56(8)
C6	.C8_h	3.556(8)	H1	.C2	2.36(7)
C7	.C1	3.502(6)	H1	.C6	3.09(8)
C7	.C6_e	3.375(8)	H1	.C7	2.50(6)
C7	.F4_g	3.121(5)	H1	.H7	2.3200
C7	.C1_e	3.506(7)	H1	.S1_e	2.89(7)
C8	.C2_e	3.581(7)	H7	.F4_g	2.6700
C8	.C10	2.311(7)	H7	.F5_g	2.7300
H7	.N1	2.4000	H12A	.F1_f	2.7400
H7	.C11	2.7600	H12B	.S1	3.0900
H7	.H1	2.3200	H12B	.F2_m	2.5300
H7	.N2_e	2.8400	H12C	.Br1	2.9000
H11	.Br1	3.0800	H12C	.C10	2.7100
H11	.C7	2.7900	H12C	.Br1_n	3.1800
H12A	.S1	2.9100			

Table S9 - Hydrogen Bonds (Angström, Degs.) for (II)

N1	--	H1	..	F1	0.83(7)	2.29(6)	2.750(5)	116(6)	.
C12	--	H12B	..	F2	0.9600	2.5300	3.135(7)	121.00	1_565
C12	--	H12C	..	Br1	0.9600	2.9000	3.365(6)	111.00	.

Translation of Symmetry Code to Equiv. Pos

a	=	[1564.00]	=	[1_564]	=	x,1+y,-1+z
b	=	[2554.00]	=	[2_554]	=	1/2+x,-y,-1/2+z
c	=	[2453.00]	=	[2_453]	=	-1/2+x,-y,-3/2+z
d	=	[2464.00]	=	[2_464]	=	-1/2+x,1-y,-1/2+z
e	=	[2454.00]	=	[2_454]	=	-1/2+x,-y,-1/2+z
f	=	[2555.00]	=	[2_555]	=	1/2+x,-y,1/2+z
g	=	[1554.00]	=	[1_554]	=	x,y,-1+z
h	=	[2455.00]	=	[2_455]	=	-1/2+x,-y,1/2+z
i	=	[1546.00]	=	[1_546]	=	x,-1+y,1+z
j	=	[1545.00]	=	[1_545]	=	x,-1+y,z
k	=	[1556.00]	=	[1_556]	=	x,y,1+z
l	=	[2556.00]	=	[2_556]	=	1/2+x,-y,3/2+z
m	=	[1565.00]	=	[1_565]	=	x,1+y,z
n	=	[2565.00]	=	[2_565]	=	1/2+x,1-y,1/2+z

CCDC_2027086. Crystallographic data for the structures reported in this paper will be available from the Cambridge Crystallographic Data Centre.