Structural study of *N*-(1,3-benzothiazol-2-yl)-4-halobenzenesulfonylhydrazides: Hirshfeld Surface analysis and PIXEL calculations

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Supplementary data

Table S1. Crystal data for compounds

	(**1**: X = F)	(**1**: X = Cl)	(**1**: X = Br)
Crystal data			
Chemical formula	$C_{13}H_{10}FN_3O_2S_2$	$C_{13}H_{10}ClN_3O_2S_2$	$C_{13}H_{10}BrN_3O_2S_2$
M_r	323.36	339.81	384.27
Crystal system, space group	Monoclinic, $P2_1/c$	Tetragonal, $P\bar{4}2_1c$	Tetragonal, $P\bar{4}2_1c$
Temperature (K)	100	106	100
a, b, c (Å)	10.8425 (2), 28.6379 (5), 8.8519 (2)	26.2216 (3), 26.2216 (3), 8.9127 (3)	26.2525 (4), 26.2525 (4), 9.0132 (4)
α, β, γ (°)	90, 90.906 (2), 90	90, 90, 90	90, 90, 90
V (Å^3)	2748.23 (9)	6128.1 (2)	6211.8 (3)
Z	8	16	16
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.41	0.53	6.19
Crystal size (mm)	0.25 × 0.18 × 0.05	0.12 × 0.03 × 0.03	0.12 × 0.03 × 0.02
Data collection			
Diffractometer	Rigaku FRE+ equipped with HF Varimax confocal mirrors and an AFC10 goniometer and HG Saturn 724+ detector	ROD, Synergy Custom system, HyPix	ROD, Synergy Custom system, HyPix
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.38.41 (Rigaku Oxford Diffraction, 2015) Empirical absorption	Multi-scan *CrysAlis PRO* 1.171.42.51a (Rigaku Oxford Diffraction, 2022) Empirical	Multi-scan *CrysAlis PRO* 1.171.42.64a (Rigaku Oxford Diffraction, 2022) Empirical absorption

	correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.641, 1.000	0.877, 1.000	0.469, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17672, 6274, 5678	69206, 7910, 6518	39123, 5760, 4748
R_{int}	0.017	0.073	0.104
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649	0.676	0.610
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.119, 1.05	0.046, 0.122, 1.06	0.041, 0.102, 1.04
No. of reflections	6274	7910	5760
No. of parameters	395	379	379
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	1.30, -0.59	0.53, -0.35	0.55, -0.65
Absolute structure	–	Flack x determined using 2495 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).	Flack x determined using 1793 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	–	0.00 (2)	-0.002 (18)

Computer programs: *CrystalClear*-SM Expert 3.1 b27 (Rigaku, 2013), *CrysAlis PRO* 1.171.42.51a (Rigaku OD, 2022), *CrysAlis PRO* 1.171.38.41 (Rigaku OD, 2015), *OSCAIL* (McArdle *et al.*, 2004), SHELXT (Sheldrick, 2015a), ShelXle (Hübschle *et al.*, 2011) *SHELXL2014*/7 (Sheldrick, 2015b), *SHELXL2018*/1 (Sheldrick, 2018), *Mercury* (Macrae *et al.*, 2006), *SHELXL2014*/17 (Sheldrick, 2015b) *PLATON* (Spek, 2009).

Table S2. Selected Torsion angles (°)

Torsion Angle	(1: X = F)	(1: X = Cl)	(1: X = Br)
C12-N121-N122-S22	103.89(17)	107.4(3)	106.1(5)
C121-S12-N122-N121	58.40(16)	55.3(3)	56.1(4)
C22-N221-N222-S22	106.84(19)	96.5(4)	95.8(5)
C221-S22-N222-N221	70.14(17)	74.6(4)	74.8(4)

Table S3. Geometric parameters (Å, °) for the π(I)···π(J) interactions

	Cg(I)···Cg(J)	Cg···Cg	α	CgI$_{perp}$	CgJ$_{perp}$	Sym code	Slippage
(1: X = 4-F)	Cg(2)···Cg(7)	3.9448(15)	9.35(12)	3.4387(10)	3.5588(10)	x,y,z	1.702
(1: X = 4-F)	Cg(3)···Cg(5)	3.9711(11)	7.95(9)	3.3440(8)	3.5291(8)	x,y,z	1.852
(1: X = 4-F)	Cg(3)···Cg(6)	4.0113(12)	8.15(10)	3.3376(8)	3.6097(8)	x,y,z	1.749
(1: X = 4-F)	Cg(5)···Cg(3)	3.9710(11)	7.95(9)	3.5129(8)	3.3439(8)	x,y,z	2.142
(1: X = 4-F)	Cg(6)···Cg(3)	4.0112(12)	8.15(10)	3.6097(9)	3.3375(8)	x,y,z	2.225
(1: X = 4-F)	Cg(6)···Cg(7)	3.9447(15)	9.35(12)	3.3387(10)	3.4387(10)	x,y,z	1.933
(1: X = 4-F)	Cg(5)···Cg(7)	3.6345(12)	16.76(10)	3.4741(8)	3.5748(9)	x,y,1+ z	0.656
(1: X = 4-F)	Cg(7)···Cg(5)	3.6345(12)	16.76(10)	3.5748(9)	3.4741(8)	x,y,-1+ z	1.068
(1: X = 4-F)	Cg(7)···Cg(6)	3.9187(12)	16.53(11)	3.5720(9)	3.1023(9)	x,y,-1+ z	2.394
(1: X = 4-Cl)	Cg(2)···Cg(7)	4.202(2)	4.2(2)	3.2976(14)	3.3787(19)	x,y,z	2.498
(1: X = 4-Cl)	Cg(7)···Cg(1)	4.202(2)	4.2(2)	3.3791(19)	3.2976(14)	x,y,z	2.604
(1: X = 4-Cl)	Cg(2)···Cg(7)	3.818(2)	3.0(2)	3.4291(16)	3.3890(19)	x,y,z	1.758
(1: X = 4-Cl)	Cg(7)···Cg(2)	3.818(2)	3.0(2)	3.3894(19)	3.4292(16)	x,y,z	1.679
(1: X = 4-Cl)	Cg(3)···Cg(5)	3.900(2)	0.3(2)	3.4217(17)	3.4267(16)	x,y,z	1.863
(1: X = 4-Cl)	Cg(5)···Cg(3)	3.901(2)	0.3(2)	3.4267(16	3.4217(17)	x,y,z	1.872
(1: X = 4-Cl)	Cg(3)···Cg(6)	3.893(3)	1.5(2)	3.4059(17)	3.4530(19)	x,y,z	1.798
(1: X = 4-Cl)	Cg(6)···Cg(3)	3.893(3)	1.5(2)	3.4530(19)	3.4059(17)	x,y,z	1.885
(1: X = 4-Cl)	Cg(5)···Cg(7)	3.831(8)	29.3(2)	3.4471(16)	3.8135(19)	x,y,-1+ z	
(1: X = 4-Cl)	Cg(7)···Cg(5)	3.831(8)	29.3(2)	3.8132(19)	3.4471(16)	x,y,1+ z	
(1: X = 4-Br)	Cg(2)···Cg(7)	3.788(3)	2.3(3)	3.410(2)	3.378(2)	x,y,z	1.713
(1: X = 4-Br)	Cg(3)···Cg(5)	3.947(3)	1.9(3)	3.419(2)	3.438(2)	x,y,z	1.938
(1: X = 4-Br)	Cg(3)···Cg(6)	3.909(3)	3.1(3)	3.399(2)	3.498(2)	x,y,z	1.744
(1: X = 4-Br)	Cg(5)···Cg(3)	3.946(3)	1.9(3)	3.438(2)	3.438(2)	x,y,z	1.972
(1: X = 4-Br)	Cg(5)···Cg(7)	3.797(3)	28.5(3)	3.385(2)	3.780(2)	x,y,1+ z	
(1: X = 4-Br)	Cg(6)···Cg(2)	3.909(3)	3.1(3)	3.498(2)	3.399(2)	x,y,z	1.931
(1: X = 4-Br)	Cg(7)···Cg(2)	3.788(3)	2.3(3)	3.378(2)	3.410(2)	x,y,z	1.649
(1: X = 4-Br)	Cg(7)···Cg(5)	3.797(3)	28.5(3)	3.780(2)	3.385(2)	x,y,-1+ z	

Atoms in rings:

Ring (1): S(11) --> C(12) --> N(13) --> C(13A) --> C(17A) ->

Ring (2):   C(13A) --> C(14) --> C(15) --> C(16) --> C(17) --> C(17A) -->
Ring (3):   C(121) --> C(122) --> C(123) --> C(124) --> C(125) --> C(126) -->
Ring (5):   S(21) --> C(22) --> N(23) --> C(23A) --> C(27A)
Ring (6:)   C(23A) --> C(24) --> C(25) --> C(26) --> C(27) --> C(27A) -->
Ring (7):   C(221) --> C(222) --> C(223) --> C(224) --> C(225) --> C(226) -->

Table S4. Assumed molecular pairs formed from intermolecular interactions in compounds (1: X = Cl and Br) on comparisons with confirmed interactions in (1: X = F)

			(1: X = Cl	(1: X = Br)	Form of molecular pair
Comparison	Symmetry code of partner to molecule at *x,y,z*	Interactions (close contacts) in (1:X = Cl or Br)	Distance (Å) angle (^{o})	Distance (Å) angle (^{o})	
Equivalent to Motif I in (**1**:X = F) Mol 1···Mol 2	*x, y, z*	N121 – H121···N23 N221 – H221·· N13 C124- X1---π(6) π2··· π7 π3··· π5 π3···π6	2.00 ; 166 2.07; 149 3.718(2);131 3.818(2) 3.900(2) 3.893(3)	2.00; 166 2.10; 145 3.824(3); 131 3.788(3) 3.497(3) 3.909(3)	Unsymmetric R$^2_2$(8)dimer
Equivalent to Motif III in (**1**:X = F) Mol 1···Mol 1	*1.5-y,1.5-x,0.5+z*	N122 – H122 ··· O122 C17-H17---π(1)	2.11[f]; 147 [g] 2.83 [h];131[i]	2.37; 127 2.83; 131	Unsymmetric cyclic dimer
Equivalent to Motifs **IVa** /**IVb** Mol 2···Mol 2	*x, y*, 1 + z *x, y*, - 1 + z	π5··· π7 π7·· π5	3.4471(16) 3.8135(19)	3.385(2)/ 3.780(2)	Unsymmetric linear dimer
Not in (**1**:X = F)	0.5+y,-0.5+y, 0.5+z	C26-H26---X1	2.81; 148	2.92; 148	Unsymmetric acyclic dimer