SUPPLEMENTARY MATERIALS

1,4-Diiodotetrafluorobenzene 3,5-di-(pyridin-4-yl)-1,2,4-thiadiazole <1/1>

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Figure S1 Solid-state FT-IR spectrum of compound **1** (500–3500 cm^{-1}, KBr pellet).

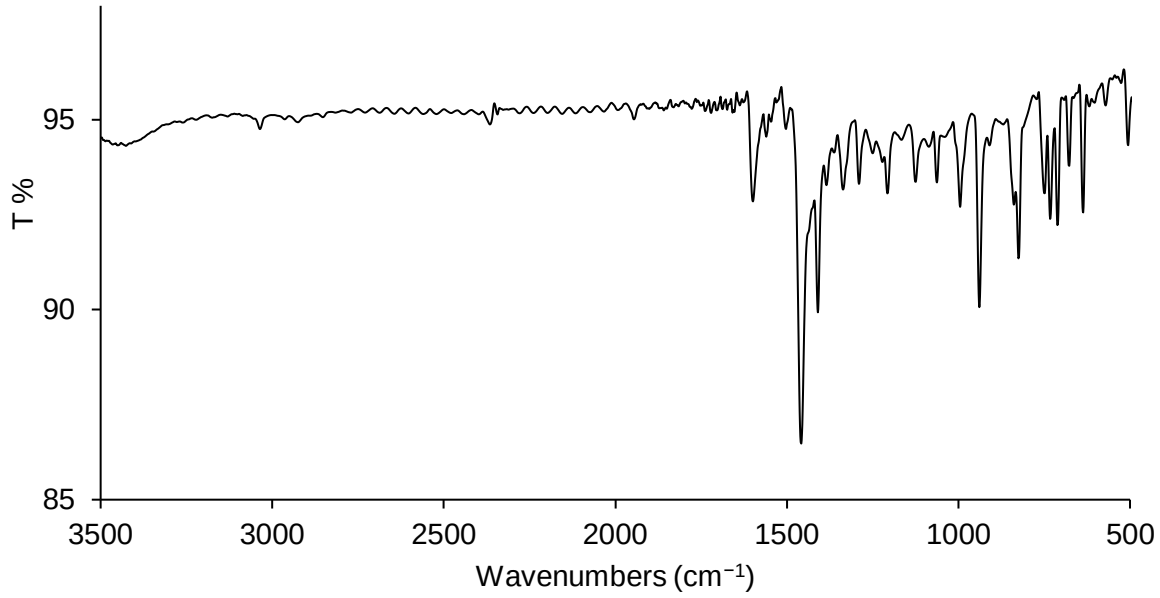

Table S1 Crystal data and structure refinement parameters for compound **1**.

Empirical formula	$C_{18}H_8F_4I_2N_4S$
Formula weight	642.14
Temperature/K	173(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	5.6690(4)
b/Å	12.3300(9)
c/Å	14.1339(9)
α/°	91.644(6)
β/°	96.314(6)
γ/°	92.400(6)
Volume/$Å^3$	980.54(12)
Z	2
ρ_{calc} / g·cm^{-3}	2.175
μ/mm^{-1}	3.363
Crystal size/mm^3	0.40 × 0.09 × 0.07
Radiation	Mo*K*α (λ = 0.71073)
2θ range for data collection/°	4.326 to 54.968
Index ranges	-7 ≤ h ≤ 7, -15 ≤ k ≤ 15, 0 ≤ l ≤ 18
Data/restraints/parameters	4439/0/263
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0333, wR_2 = 0.0873
Final R indexes [all data]	R_1 = 0.0450, wR_2 = 0.0960
Largest diff. peak/hole / e·$Å^{-3}$	1.03/−0.71

Table S2 Bond lengths (Å) for compound **1**.

N1–I1	2.801(5)	C8–C12	1.392(7)
N4–I2^{i}	2.947(4)	C8–C9	1.369(6)
I1–C13	2.101(4)	C8–C7	1.497(6)
I2–C16	2.091(4)	C4–C3	1.393(6)
S1–N3	1.618(4)	C4–C5	1.376(7)
S1–C6	1.708(5)	C13–C18	1.379(7)
F3–C18	1.339(5)	C13–C14	1.393(6)
F4–C17	1.350(5)	C3–C6	1.489(6)
F1–C14	1.347(5)	C3–C2	1.376(7)
F2–C15	1.338(5)	C12–C11	1.381(7)
N3–C7	1.345(6)	C18–C17	1.371(6)
N2–C7	1.367(6)	C9–C10	1.371(7)
N2–C6	1.314(6)	C14–C15	1.374(6)
N1–C5	1.341(7)	C1–C2	1.376(7)
N1–C1	1.318(7)	C16–C17	1.373(6)
N4–C10	1.343(7)	C16–C15	1.402(6)
N4–C11	1.332(6)		

Symmetry code: ^{i} = 2+x, −1+y, −1+z.

Table S3 Bond angles (°) for compound **1**.

N1–I1–C13	177.4(2)	F1–C14–C13	120.5(4)
N4–I2^{i}–C16^{i}	168.3(2)	F1–C14–C15	118.1(4)
N3–S1–C6	93.2(2)	C15–C14–C13	121.4(4)
C7–N3–S1	107.6(3)	N1–C1–C2	124.1(5)
C6–N2–C7	107.5(4)	C17–C16–I2	122.7(3)
C1–N1–C5	116.7(4)	C17–C16–C15	116.9(4)
C11–N4–C10	116.9(4)	C15–C16–I2	120.3(3)
C12–C8–C7	121.3(4)	F4–C17–C18	118.5(4)
C9–C8–C12	118.4(4)	F4–C17–C16	119.7(4)
C9–C8–C7	120.3(4)	C18–C17–C16	121.8(4)
C5–C4–C3	117.8(5)	N3–C7–N2	119.1(4)
C18–C13–I1	121.9(3)	N3–C7–C8	120.3(4)
C18–C13–C14	116.8(4)	N2–C7–C8	120.6(4)
C14–C13–I1	121.3(3)	F2–C15–C14	119.0(4)
C4–C3–C6	119.9(4)	F2–C15–C16	119.9(4)
C2–C3–C4	118.6(4)	C14–C15–C16	121.1(4)
C2–C3–C6	121.5(4)	N4–C10–C9	123.8(5)
N1–C5–C8	124.0(5)	N2–C6–S1	112.6(3)
C11–C12–C13	118.9(4)	N2–C6–C3	124.4(4)
F3–C18–C17	119.3(4)	C3–C6–S1	123.0(3)
F3–C18–C13	118.8(4)	C1–C2–C3	118.7(5)
C17–C18–C10	122.0(4)	N4–C11–C12	123.1(5)
C8–C9–C10	118.9(5)		

Symmetry code: ^{i} = 2+x, −1+y, −1+z.