Mixed radical iodine charge-transfer salts of dithiadiazolyl diradicals. Structural characterization of the pyridine-bridged 2:1 salt 2,6-[(S2N2C)C5H3N(CN2S2)](2)[I]

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Table S1 Crystal and refinement data for $[P\text{-}2,6\text{-}S]_2[I]$.

formula	$IS_8N_{10}C_{14}H_6$
fw	348.83
crystal size, mm	0.51 x 0.11 x 0.08
crystal color	black
crystal mount	on glass fiber by epoxy
a, Å	3.434(3)
b, Å	9.8914(9)
c, Å	30.803(4)
β, deg	91.52(3)
V, Å^3	1045.9(9)
cell detn, refls	25
cell detn, 2θ range, deg	14-18
d(calcd), g cm^{-3}	2.22
space group	$P2_1/c$
Z	2
F_{000}	681.87
radiation	MoK_α, graphite monochromated
λ, Å	0.71073
temp, K	293
linear abs coeff,mm^{-1}	2.31
diffractometer	Enraf-Nonius CAD-4
scan technique	θ-2θ
scan speed, deg min^{-1}	4-16 (in omega)
scan width, deg	$1.0 + 0.35\tan\theta$
2θ range, deg	4-50
h, k, l ranges	0,4; 0,11; -36,36
exposure time, hrs	53.5
std refl indices	4,0,-8; 0,3,-7; 0,1,11
drift of stds, %	1.3
absorption correction	empirical psi scans

absorption, range	0.91-1.00
refl meas	2154
unique refls	1823
R for merge	0.066
data with $I > 3\sigma(I)$	1163
solution method	Direct Methods
parameters refined	154
$R(F)$, $R_w(F)$	0.047, 0.081
GOF	1.36
p, $w^{-1} = [\sigma^2(I)+pI^2]/4F^2$	0.05
largest Δ/σ	0.000
extinction correction	none
final diff map, e A^{-3}	-0.6(1), +0.5(1)
programs	NRC386 (PC version ofNRCVAX)*
scattering factors	Internat. Tables for Crystallography Vol 4
H atom treatment	idealized positions (C-H = 0.95Å)

*PC version of NRCVAX, an interactive program system for structure analysis; see E.J. Gabe, Y. LePage, J.P. Charland, F.L. Lee, and P.S. White, *J. Appl. Cryst.* **22**, 383 (1989).

SPECIAL NOTE: During the refinement of the anisotropic temperature factors of I1 and I2, they were constrained to be equivalent due a large correlation. Iodine position occupancies were determined (I1/I2 = 0.3974/0.3013) during isotropic refinement and locked at those values prior to anisotropic refinement.

Table S2 Bond distances (Å) and angles (°) for $[P\text{-}2,6\text{-}S]_2[I]$. ESDs refer to the last digit printed.

Distances		Angles	
S(1)-S(2)	2.065(3)	S(2)-S(1)-N(1)	93.6(3)
S(1)-N(1)	1.607(9)	S(1)-S(2)-N(2)	95.2(3)
S(2)-N(2)	1.613(8)	S(4)-S(3)-N(3)	94.2(3)
S(3)-S(4)	2.082(4)	S(3)-S(4)-N(4)	94.6(3)
S(3)-N(3)	1.629(8)	S(1)-N(1)-C(1)	117.3(6)
S(4)-N(4)	1.635(8)	S(2)-N(2)-C(1)	114.7(6)
N(1)-C(1)	1.325(11)	S(3)-N(3)-C(7)	114.6(6)
N(2)-C(1)	1.358(10)	S(4)-N(4)-C(7)	113.4(6)
N(3)-C(7)	1.313(12)	C(2)-N(5)-C(6)	117.6(7)
N(4)-C(7)	1.335(12)	N(1)-C(1)-N(2)	119.1(7)
N(5)-C(2)	1.351(10)	N(1)-C(1)-C(2)	119.8(7)
N(5)-C(6)	1.345(11)	N(2)-C(1)-C(2)	121.0(7)
C(1)-C(2)	1.443(11)	N(5)-C(2)-C(1)	117.9(7)
C(2)-C(3)	1.393(12)	N(5)-C(2)-C(3)	121.9(8)
C(3)-C(4)	1.375(13)	C(1)-C(2)-C(3)	120.2(7)
C(4)-C(5)	1.348(15)	C(2)-C(3)-C(4)	119.7(8)
C(5)-C(6)	1.382(13)	C(3)-C(4)-C(5)	117.7(8)
C(6)-C(7)	1.483(13)	C(4)-C(5)-C(6)	121.6(9)
		N(5)-C(6)-C(5)	121.4(8)
		N(5)-C(6)-C(7)	117.5(8)
		C(5)-C(6)-C(7)	121.1(8)
		N(3)-C(7)-N(4)	123.3(8)
		N(3)-C(7)-C(6)	116.5(8)
		N(4)-C(7)-C(6)	120.1(8)

Table S3 Intermolecular S---I contacts (Å) for $[P\text{-}2,6\text{-}S]_2[I]$. ESDs refer to the last digit printed.

S3---I1	(at 1 - x, 0.5 + y, 0.5 - z)	3.479(3)
S3---I2	(at 2 - x, 0.5 + y, 0.5 - z)	3.594(7)
S3---I2	(at x - 1, 1.5 - y, 0.5 + z)	3.428(7)
S4---I1	(at 1 - x, 0.5 + y, 0.5 - z)	3.748(3)
S4---I2	(at 2 - x, 0.5 + y, 0.5 - z)	3.842(6)
S4---I2	(at x - 1, 1.5 - y, 0.5 + z)	3.716(6)

Table S4 Anisotropic temperature factors, u(i,j)*100, for $[P\text{-}2,6\text{-}S]_2[I]$. ESDs refer to the last digit printed.

	u11(U)	u22	u33	u12	u13	u23
I1	3.2 (3)	3.55(6)	3.02(6)	-0.22(24)	-0.34(21)	-0.22(4)
I2	3.2 (3)	3.55(6)	3.02(6)	-0.22(24)	-0.34(21)	-0.22(4)
S1	10.8 (3)	2.33(12)	3.32(13)	0.60(14)	-2.19(15)	-0.73(9)
S2	5.97(17)	3.16(12)	2.65(11)	0.30(12)	-0.79(11)	-0.17(9)
S3	8.78(23)	4.32(14)	2.79(12)	2.44(15)	0.11(14)	-0.50(10)
S4	6.47(19)	3.69(14)	3.74(14)	1.78(13)	-0.28(13)	-0.22(10)
N1	5.3 (6)	1.9 (3)	5.7 (5)	0.2 (4)	-1.7 (4)	-0.1 (3)
N2	3.0 (4)	2.3 (3)	3.6 (4)	0.2 (3)	-0.2 (3)	-0.2 (3)
N3	5.6 (5)	4.3 (4)	2.8 (4)	1.5 (4)	0.5 (4)	0.4 (3)
N4	6.3 (6)	3.9 (4)	2.1 (4)	1.2 (4)	0.8 (4)	0.2 (3)
N5	1.6 (4)	3.1 (4)	3.4 (4)	0.1 (3)	-0.7 (3)	0.3 (3)
C1	4.1 (5)	2.7 (4)	2.0 (4)	0.1 (4)	-1.1 (4)	0.2 (3)
C2	1.0 (4)	2.4 (4)	3.7 (5)	0.6 (3)	-0.2 (4)	0.3 (3)
C3	2.5 (5)	3.3 (5)	5.6 (6)	-0.1 (4)	0.2 (5)	0.8 (4)
C4	2.6 (5)	5.0 (6)	4.1 (5)	0.3 (5)	0.6 (4)	2.0 (4)
C5	2.8 (5)	5.1 (6)	3.6 (5)	0.5 (5)	-0.6 (4)	1.8 (4)
C6	2.1 (5)	3.6 (5)	3.2 (4)	1.1 (4)	-0.3 (4)	-0.1 (4)
C7	3.0 (5)	4.0 (5)	3.5 (5)	1.1 (4)	0.5 (4)	0.1 (4)

Anisotropic temperature factors are of the form:

$$\exp[-2\pi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hkU_{12}a^*b^* + 2hlU_{13}a^*c^* + 2klU_{23}b^*c^*)].$$

Figure S1 ORTEP drawing of the asymmetric unit in $[P\text{-}2,6\text{-}S]_2[I]$.