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Molecular Conductors from Neutral-Radical Charge-Transfer Salts

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Table S1 Crystal and Refinement Data

formula	$S_4N_{4.16}C_2H_2$	$S_2N_2CHI_{0.18}$
fw	212.4	128.20
crystal size, mm	0.20 x 0.30 x 0.68	0.20 x 0.20 x 0.65
crystal color	black	black
crystal mount	in epoxy-filled capillary	in epoxy-filled capillary
a, Å	6.816(3)	14.132(16)
b, Å	13.940(2)	14.132(16)
c, Å	14.403(3)	3.352(5)
α, deg	116.830(14)	90
β, deg	98.64(3)	90
γ, deg	99.18(3)	120
V, Å^3	1166.5(6)	579.8(1)
cell detn, refls	25	25
cell detn, 2θ range, deg	13-25	16-18
d(calcd), g cm^{-3}	1.81	2.203
space group	$P\bar{1}$	$P6_1$
Z	6	6
F_{000}	645.1	376.39
radiation	MoK_α, graphite monochromated	
λ, Å	0.71073	
temp, K	293	
diffractometer	Enraf-Nonius CAD-4	
scan technique	θ-2θ	
linear abs coeff, mm^{-1}	1.10	2.38
scan speed, deg min^{-1}	4-16 (in omega)	4-16 (in omega)
scan width, deg	1.0 + 0.35tanθ	1.0 + 0.35tanθ
2θ range, deg	4-50	4-50
h, k, l ranges	-8,8; 0,19; 0,22	0,14; 0,14; 0,3
exposure time, hrs	53.4	15.6

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std refl indices	-2,1,-1; 0,0,5; 1,3,2	-4,2,-1; 5,0,0; 0,5,0
drift of stds, %	0.9	1.1
absorption correction	empirical psi-scans	empirical psi scans
absorption, range	0.80 - 1.00	0.517 - 0.999
refl meas	8176	2324
unique refls	4088	400
R for merge	0.04	0.091
data with $I > 3\sigma(I)$	1746	198
solution method	Direct Methods	SHELX
parameters refined	273	32
$R(F^2)$, $R_w(F^2)$[a]	0.045,0.054	0.074,0.115
GOF	1.31	1.94
p, $w^{-1}=[\sigma^2(I)+pI_2]/4F^2$	0.03	0.05
largest Δ/σ	0.004	0.017
extinction correction	none	none
final diff map, e $Å^{-3}$	+0.50(9),-0.35(9)	-0.40(13) +0.51(13)
programs	NRC386 (PC version of NRCVAX)[b]	
scattering factors	Internat. Tables for Crystallography Vol 4	
H atom treatment	idealized positions (C-H = 0.95A)	

[a] $R = [\Sigma||F_o| - |F_c||]/[\Sigma|F_o|]$; $R_w = \{[\Sigma w||F_o| - |F_c||^2]/[\Sigma(w|F_o|^2)]\}^{1/2}$

[b] 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).

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Table S2 Interatomic distances (Å) and angles (deg) in $[HCN_2S_2]_2[N_2]_{0.08}$.

Distances

S(1)-S(2)	2.059(4)	S(11)-N(11)	1.636(9)
S(1)-N(1)	1.656(9)	S(12)-N(12)	1.637(9)
S(2)-N(2)	1.626(10)	N(1)-C(1)	1.333(16)
S(3)-S(4)	2.058(4)	N(2)-C(1)	1.328(16)
S(3)-N(3)	1.621(9)	N(3)-C(2)	1.335(16)
S(4)-N(4)	1.639(9)	N(4)-C(2)	1.311(16)
S(5)-S(6)	2.055(4)	N(5)-C(3)	1.334(15)
S(5)-N(5)	1.658(9)	N(6)-C(3)	1.334(16)
S(6)-N(6)	1.613(9)	N(7)-C(4)	1.335(16)
S(7)-S(8)	2.070(4)	N(8)-C(4)	1.308(15)
S(7)-N(7)	1.629(10)	N(9)-C(5)	1.330(15)
S(8)-N(8)	1.639(9)	N(10)-C(5)	1.323(14)
S(9)-S(10)	2.065(4)	N(11)-C(6)	1.338(14)
S(9)-N(9)	1.643(9)	N(12)-C(6)	1.301(15)
S(10)-N(10)	1.634(9)	N(98)-N(98)a	1.17
S(11)-S(12)	2.065(4)	N(98)-N(99)	1.13

Angles

S(2)-S(1)-N(1)	95.2(4)	S(5)-N(5)-C(3)	112.2(7)
S(1)-S(2)-N(2)	95.2(4)	S(6)-N(6)-C(3)	114.4(7)
S(4)-S(3)-N(3)	95.5(4)	S(7)-N(7)-C(4)	110.8(8)
S(3)-S(4)-N(4)	94.9(3)	S(8)-N(8)-C(4)	111.5(8)
S(6)-S(5)-N(5)	95.1(3)	S(9)-N(9)-C(5)	111.9(7)
S(5)-S(6)-N(6)	95.1(3)	S(10)-N(10)-C(5)	113.1(8)
S(8)-S(7)-N(7)	95.6(4)	S(11)-N(11)-C(6)	112.2(7)
S(7)-S(8)-N(8)	94.9(3)	S(12)-N(12)-C(6)	112.8(7)
S(10)-S(9)-N(9)	95.4(4)	N(1)-C(1)-N(2)	124.7(10)
S(9)-S(10)-N(10)	94.6(4)	N(3)-C(2)-N(4)	125.7(10)
S(12)-S(11)-N(11)	94.8(3)	N(5)-C(3)-N(6)	123.2(9)
S(11)-S(12)-N(12)	95.0(3)	N(7)-C(4)-N(8)	127.2(11)
S(1)-N(1)-C(1)	111.6(8)	N(9)-C(5)-N(10)	124.9(10)
S(2)-N(2)-C(1)	113.2(8)	N(11)-C(6)-N(12)	125.3(9)
S(3)-N(3)-C(2)	111.9(8)		
S(4)-N(4)-C(2)	112.0(8)		

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Table S3 Interatomic distances (Å) and angles (deg) in $[HCN_2S_2]_6[I_{1.1}]$.

Distances

S(1)-S(2)	2.051(11)
S(1)-N(1)	1.65(3)
S(2)-N(2)	1.654(24)
N(1)-C(1)	1.34(4)
N(2)-C(1)	1.31(4)

Angles

S(2)-S(1)-N(1)	95.4(10)
S(1)-S(2)-N(2)	95.3(8)
S(1)-N(1)-C(1)	111.2(19)
S(2)-N(2)-C(1)	112.1(20)
N(1)-C(1)-N(2)	125(3)

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Table S4 Table of u(i,j) values (*100) for $[HCN_2S_2]_2[N_2]_{0.08}$. ESDs refer to the last digit printed.

	u11(U)	u22	u33	u12	u13	u23
S1	4.74(21)	3.73(18)	4.26(18)	-0.84(16)	0.58(16)	1.78(14)
S2	5.50(22)	3.62(19)	4.12(18)	0.36(17)	1.47(16)	1.56(14)
S3	6.58(24)	2.95(17)	4.62(19)	1.30(17)	1.64(18)	1.99(14)
S4	4.53(20)	3.62(18)	3.78(17)	0.74(16)	0.40(15)	1.70(14)
S5	4.27(20)	3.65(18)	4.54(18)	-0.05(16)	0.77(15)	2.08(14)
S6	5.12(20)	3.29(18)	4.24(18)	1.02(16)	0.95(16)	2.08(14)
S7	5.59(22)	3.68(19)	4.78(19)	1.00(17)	0.88(17)	2.04(15)
S8	4.64(20)	4.38(19)	3.22(16)	0.27(17)	0.94(15)	1.92(14)
S9	5.22(22)	4.08(21)	3.95(18)	0.74(19)	1.69(17)	1.89(15)
S10	4.16(20)	3.55(19)	3.95(18)	0.31(17)	0.44(15)	1.46(14)
S11	4.72(21)	3.73(19)	4.33(18)	0.74(18)	0.70(16)	2.12(15)
S12	4.62(20)	3.30(18)	3.38(17)	0.68(16)	1.14(15)	1.29(13)
N1	5.0 (7)	4.5 (7)	3.6 (6)	0.5 (6)	0.1 (5)	2.1 (5)
N2	4.4 (7)	4.4 (6)	5.3 (6)	1.3 (6)	1.7 (5)	2.2 (5)
N3	7.5 (8)	3.9 (6)	3.7 (6)	0.5 (6)	1.8 (6)	1.4 (5)
N4	5.7 (7)	3.6 (6)	4.6 (6)	0.4 (6)	1.1 (5)	2.1 (5)
N5	5.7 (7)	4.7 (7)	3.0 (6)	1.2 (6)	0.9 (5)	2.0 (5)
N6	8.1 (8)	2.9 (6)	3.3 (6)	0.8 (6)	1.3 (5)	1.0 (5)
N7	5.7 (7)	5.0 (7)	5.0 (6)	0.9 (6)	0.6 (5)	3.0 (5)
N8	4.4 (6)	4.6 (6)	3.8 (6)	0.1 (5)	0.9 (5)	1.9 (5)
N9	6.5 (8)	4.7 (7)	4.2 (6)	1.5 (6)	2.1 (6)	1.6 (5)
N10	4.9 (7)	3.5 (6)	6.6 (7)	1.1 (6)	1.2 (6)	3.0 (5)
N11	3.9 (6)	3.5 (6)	3.5 (6)	0.1 (5)	0.0 (5)	1.2 (5)
N12	6.8 (8)	4.3 (6)	2.6 (5)	1.4 (6)	1.8 (5)	1.7 (5)
C1	3.6 (7)	5.4 (8)	5.6 (8)	0.5 (7)	0.0 (6)	3.9 (7)
C2	7.4 (11)	4.6 (9)	4.4 (8)	1.3 (8)	2.8 (8)	2.4 (7)
C3	5.4 (9)	4.3 (8)	3.1 (7)	0.8 (7)	0.9 (6)	0.5 (6)
C4	4.9 (9)	6.2 (10)	3.7 (7)	0.6 (8)	0.0 (6)	2.5 (7)
C5	4.4 (8)	3.2 (7)	3.2 (7)	0.9 (6)	-0.4 (6)	0.2 (5)
C6	4.5 (8)	3.1 (7)	5.9 (8)	0.5 (6)	2.5 (7)	2.5 (6)

Table S5 Table of u(i,j) values (*100) for $[HCN_2S_2]_6[I_{1.1}]$. ESDs refer to the last digit printed.

	u11(U)	u22	u33	u12	u13	u23
S1	8.1(5)	8.6(5)	7.5(7)	3.7(4)	-1.1(5)	1.1(5)
S2	8.6(6)	8.5(5)	9.7(8)	4.1(4)	-1.1(5)	2.3(6)

Anisotropic temperature factors are of the form:

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

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Figure S1 ORTEP drawings of the three non-equivalent dimers in $[HCN_2S_2]_2[N_2]_{0.08}$, showing atom numbering.

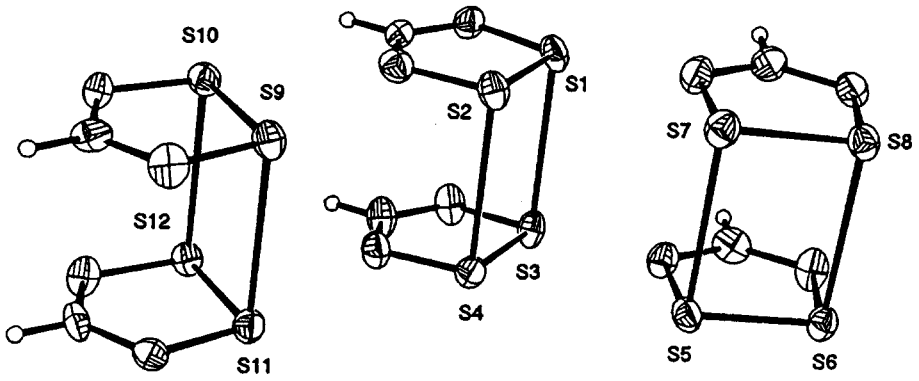

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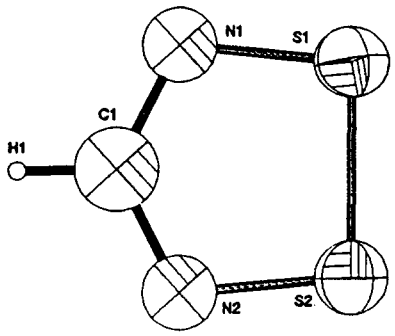
Figure S2 ORTEP drawings of the heterocyclic ring in $[HCN_2S_2]_6[I_{1.1}]$, showing atom numbering.



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