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6-Amino-4-iminio-4*H*-1,3,5-dithiazole iodide

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Key indicators

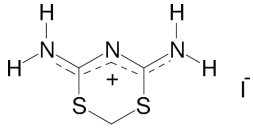
Single-crystal X-ray study
T = 150 K
Mean σ(N–C) = 0.005 Å
R factor = 0.044
wR factor = 0.109
Data-to-parameter ratio = 18.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, $C_3H_6IN_3S_2$, comprises a puckered ring that associates to the I^- anion *via* N—H···I interactions. In the asymmetric unit, two I^- anions reside on special positions (twofold rotation axes) equivalent to one complete anion per cation. The cationic charge is delocalized between the two amines, as suggested by the similar bond lengths, across the heterocyclic N atom, between these two groups.

Comment

Compound (I) is marketed as 4,6-diimino-1,3,5-dithiazolidine hydrogen iodide (Fig. 2*a*) whereas elucidation of the crystal structure reveals a delocalized cation with an I^- anion. The two resonant forms, from which the compound has been named, are shown in Fig. 2(*b*). Bond distances for the atoms between the two amines are listed in Table 2.



(I)

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis.

Crystal data

$C_3H_6N_3S_2^+\cdot I^-$
M_r = 275.13
Monoclinic, $C2/c$
a = 11.050 (2) Å
b = 18.964 (4) Å
c = 8.1307 (16) Å
β = 108.87 (3)°
V = 1612.2 (6) Å^3
Z = 8
D_x = 2.267 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5412 reflections
θ = 1.0–27.5°
μ = 4.41 mm^{-1}
T = 150 (2) K
Plate, colourless
0.35 × 0.20 × 0.08 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.307, T_{max} = 0.719
7382 measured reflections
1818 independent reflections
1726 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 27.5°
$h = -14 \rightarrow 13$
$k = -24 \rightarrow 24$
$l = -10 \rightarrow 10$

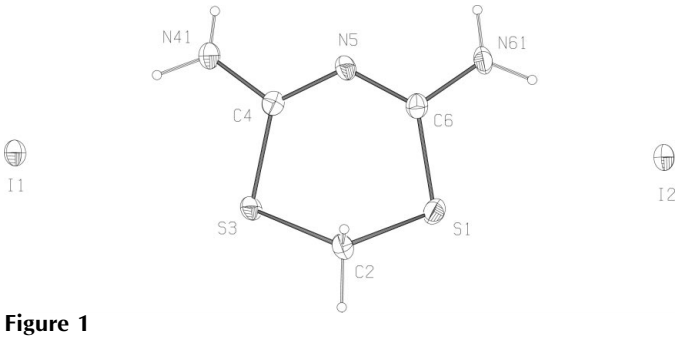


Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 50% probability displacement ellipsoids.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0850P)^2 + 0.3966P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.109$	$\Delta\rho_{max} = 2.79$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -2.70$ e Å^{-3}
1818 reflections	Extinction correction: *SHELXL*97
100 parameters	Extinction coefficient: 0.0043 (5)
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å).

C4—N41	1.302 (4)	N5—C6	1.325 (4)
C4—N5	1.325 (4)	C6—N61	1.314 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N41—H41···I1^{i}	0.74 (4)	3.13 (4)	3.786 (3)	150 (3)
N41—H42···I1	0.91 (4)	2.68 (4)	3.581 (3)	169 (4)
N61—H61···I2^{ii}	0.85 (5)	2.88 (5)	3.663 (3)	155 (4)
N61—H62···I2^{iii}	0.86 (4)	2.80 (4)	3.638 (3)	165 (4)

Symmetry codes: (i) $1-x, -y, 1-z$; (ii) $-x, -y, 1-z$; (iii) $x, y, 1+z$.

The four amine H atoms were located on difference syntheses and both displacement and positional parameters were refined, while the CH_2 H atoms were included in the refinement at calculated positions as riding models, with C—H set to 0.99 Å. The largest difference map features were close to the I^- anions.

Data collection, cell refinement and data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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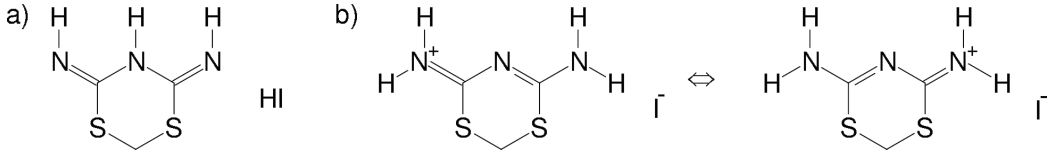

Figure 2
The structures of (*a*) the marketed configuration and (*b*) the resonant forms of (I).