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Synthesis and structure of 4,5-diphenyl-1*H*-imidazol-3-ium thiocyanate

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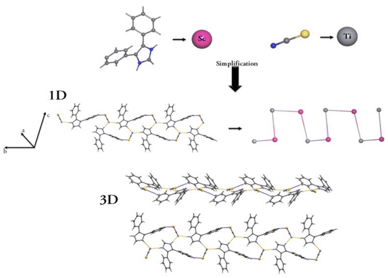
In the title molecular salt, $C_{15}H_{13}N_2^{+}\cdot SCN^{-}$, the dihedral angles between the imidazole ring and pendant phenyl groups are 51.61 (14) and 35.47 (15)°. In the crystal, the ions are linked by N—H⋯N and C—H⋯S hydrogen bonds, forming $R_2^4(16)$ loops. These units are further connected by C—H⋯π and C—S⋯π interactions into a three-dimensional supramolecular network. Hirshfeld surface analysis of the imidazolium cation shows that H⋯H (42.9%), C⋯H/H⋯C (34.9%), N⋯H/H⋯N (10.7%) and H⋯S/S⋯H (6.5%) contacts are the major contributors to the crystal packing.

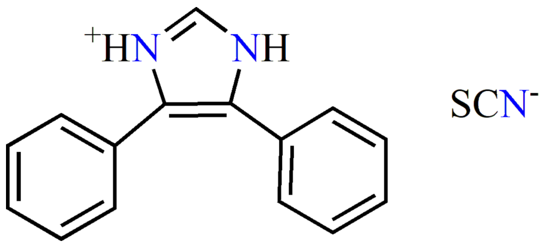


1. Chemical context

Imidazole derivatives continue to attract attention in structural and supramolecular chemistry because they combine aromatic character, amphoteric behaviour and multiple donor/acceptor sites within a compact heterocyclic framework (Chen, 2016). In their neutral form, imidazoles are widely encountered as ligands and functional organic building blocks, whereas protonated imidazolium species are particularly attractive as cationic components of molecular salts, where they can serve as efficient hydrogen-bond donors and promote the formation of extended supramolecular assemblies. Aryl substitution at the 4- and 5-positions further enlarges the π-surface of the heterocycle and can enhance weak intermolecular contacts involving aromatic rings.

A search of the Cambridge Structural Database (CSD, version 6.01 with updates to February 2026; Groom *et al.*, 2016) for the 4,5-diarylimidazole skeleton shows that this family is structurally diverse and includes neutral molecules, solvates and ionic derivatives. Representative neutral examples include 4,5-diphenyl-1*H*-imidazole (Stibrany *et al.*, 2004; Kounavi *et al.*, 2012), 2-(4,5-diphenyl-1*H*-imidazol-2-yl)phenol (Fridman *et al.*, 2009), 4-(4,5-diphenyl-1*H*-imidazol-2-yl)-benzaldehyde (Kimura *et al.*, 2002), 2,4,5-triphenyl-4,5-dihydro-1*H*-imidazole hemihydrate (Huang *et al.*, 2006).

Related salts and co-crystals further illustrate the versatility of this heterocyclic platform in the solid state. Examples include 4,5-diphenyl-2-(4-nitrophenyl)-1*H*-imidazole clathrates with water, acetic acid and dimethyl sulfoxide (Kaftory *et al.*, 1998), 2-(3-nitrophenyl)-4,5-diphenyl-1*H*-imidazol-3-ium nitrate (Zhang, 2009), and trans-2-amino-4,5-diphenyl-4,5-dihydroimidazolium nitrate derivatives (Wüstenberg *et al.*, 2023). These examples show that protonation of the imidazole ring and association with counter-ions or neutral conformers can generate a rich variety of supramolecular arrangements governed by classical hydrogen bonds and weaker aromatic contacts.



As part of our studies in this area, and in the context of our ongoing research on azole-based compounds (Bensegueni *et al.*, 2009, 2014, 2015, 2020), we now report the synthesis and structure of the title molecular salt, $C_{15}H_{13}N_2^{+}\cdot SCN^{-}$ (**I**), in order to analyse how different types of hydrogen bonds cooperate in the consolidation of the crystal packing.

2. Structural commentary

The asymmetric unit of compound (**I**) consists of one 4,5-biphenylimidazolium cation and one thiocyanate anion. The crystal structure is orthorhombic and crystallizes in the space group $P2_12_12_1$ with a well-defined absolute structure.

The cation is formed by a protonated imidazolium ring substituted at the 4- and 5-positions by two phenyl groups. The imidazolium core, defined by atoms N1/N2/C1/C2/C9, displays bond lengths of 1.319 (4) Å for N1—C1, 1.326 (4) Å for N2—C1, 1.382 (4) Å for N1—C9 and 1.386 (3) Å for N2—C2, which are consistent with charge delocalization within the aromatic imidazolium fragment (Fig. 1). The cation consists of two phenyl rings (*A* containing C3–C8 and *C* containing C10–C15) and one imidazole ring (*B*) (see supplementary figure). The interplanar angles are 51.61 (14)° for *A*/*B*, 35.47 (15)° for *B*/*C* and 54.80 (12)° for *A*/*C*.

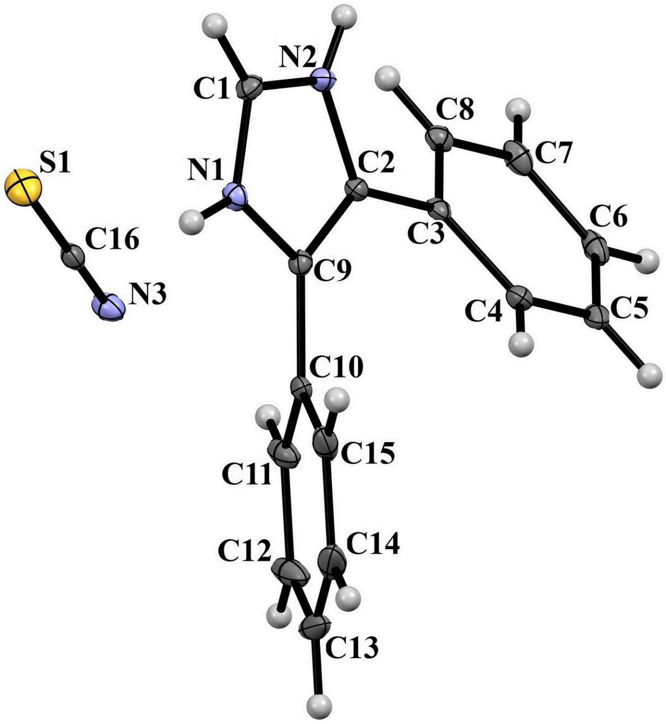


Figure 1
The molecular structure of (**I**) showing displacement ellipsoids drawn at the 50% probability level.

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the N1/C1/N2/C2/C9, C3–C8 and C10–C15 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$N3^{i}	0.86	1.98	2.835 (4)	171
N2—H2$\cdots$N3^{ii}	0.86	2.02	2.862 (3)	168
C12—H12$\cdots$S1^{iii}	0.93	2.93	3.785 (2)	155
C1—H1$A\cdots Cg3^{iv}$	0.93	2.45	3.330 (3)	158
C6—H6$\cdots Cg2^{v}$	0.93	2.93	3.581 (4)	128
C7—H7$\cdots Cg1^{vi}$	0.93	2.91	3.297 (4)	106

Symmetry codes: (i) $x + 1, y, z$; (ii) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (iv) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$; (v) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (vi) $x - 1, y, z$.

As expected, the thiocyanate anion is essentially linear, with an N3—C16—S1 bond angle of 179.4 (3)°. The corresponding bond distances, N3—C16 = 1.171 (4) Å and C16—S1 = 1.622 (3) Å, are in agreement with the expected geometry of a thiocyanate anion.

3. Supramolecular features

The crystal structure of (**I**) features three hydrogen bonds involving the thiocyanate anion as the principal acceptor. The N1—H1*N*$\cdots$N3 and N2—H2$\cdots$N3 hydrogen bonds (Table 1), with H$\cdots$N distances of 1.98 and 2.02 Å, together with the C12—H12$\cdots$S1 contact (H$\cdots$S = 2.93 Å), generate an $R_4^3(16)$ ring motif that links two cations and two anions into discrete supramolecular cycles in the crystal packing (Fig. 2). In addition to these classical hydrogen bonds, the structure features three C—H$\cdots\pi$ interactions, with each aromatic ring accepting one such interaction. The C1—H1*A*$\cdots$*Cg*3 contact, with a notably short H$\cdots$*Cg* distance of 2.45 Å, reinforces the $R_4^3(16)$ motif (Etter *et al.*, 1990). The other two bonds connect adjacent motifs into extended chains (supplementary figure).

The crystal packing also features a very weak π–π stacking interaction between the *A* and *B* aromatic rings, with a centroid–centroid separation of 4.201 (12) Å, reinforced by a C—S$\cdots$*Cg*1 contact [3.534 (2) Å, 94.96 (11)°], which links the hydrogen-bonded chains along the *a*- and *c*-axis directions and contributes to the three-dimensional supramolecular archi-

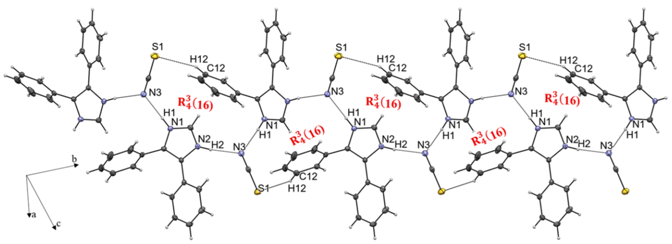


Figure 2
The crystal packing of (**I**), showing the $R_4^3(16)$ hydrogen-bonded ring motifs and the one-dimensional chain generated by N—H$\cdots$N and C—H$\cdots$S interactions.

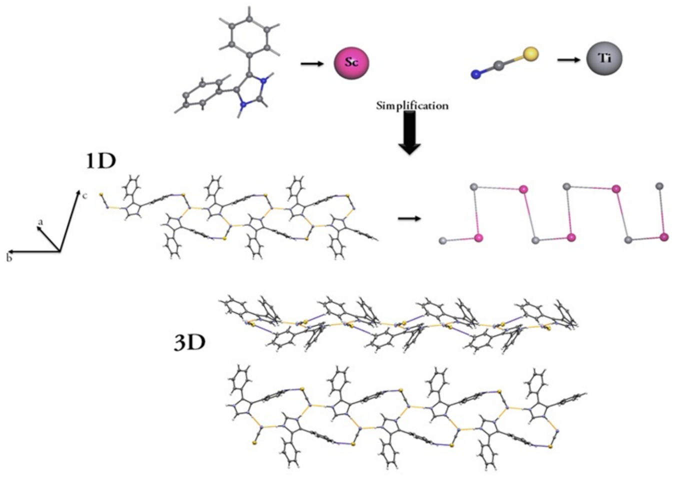


Figure 3
Simplified representation of the crystal packing showing the one-dimensional zigzag chain and its three-dimensional extension in (**I**).

tecture. Overall, these interactions produce a zigzag one-dimensional arrangement extending along the *b* axis, which is then assembled into the full three-dimensional network (Fig. 3).

4. Hirshfeld surface analysis

Hirshfeld surface (HS) analysis and the corresponding two-dimensional fingerprint plots (Fig. 4) were generated using *CrystalExplorer 21.5* (Spackman *et al.*, 2021) in order to examine the intermolecular interactions governing the crystal packing of the title salt. On the $d_{\rm norm}$-mapped Hirshfeld surface (Fig. 6), the most intense red spots are associated with the shortest intermolecular contacts, particularly those involving the thiocyanate anion. These include the N—H⋯N and C—H⋯S hydrogen bonds, as well as the C—S⋯π and C—H⋯π interactions, which play a central role in the cohesion of the ionic assembly.

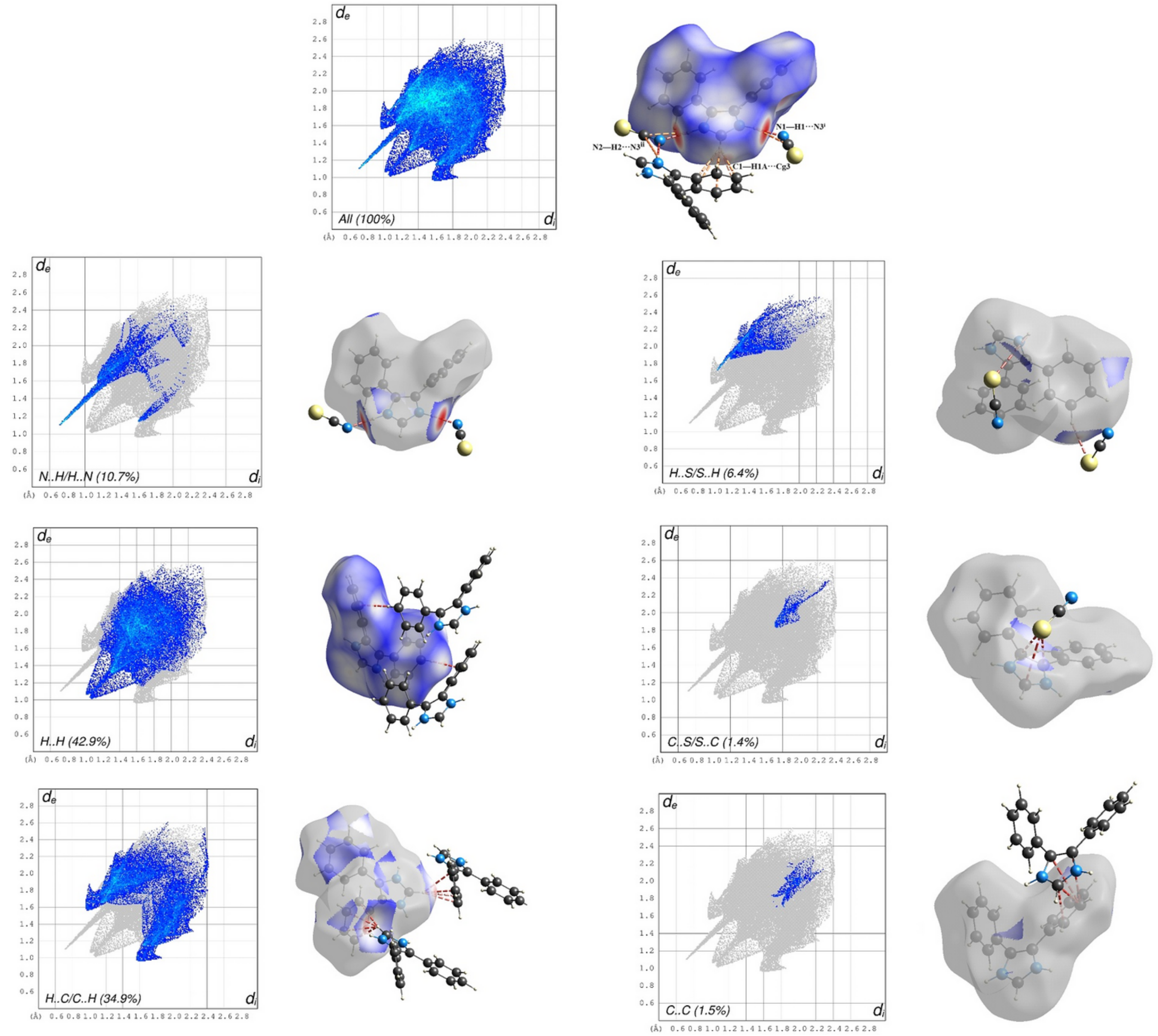


Figure 4
Hirshfeld surface mapped over $d_{\rm norm}$ and the associated fingerprint plots for (**I**), showing the percentage contributions of the different intermolecular contacts.

The two-dimensional fingerprint plots indicate that H⋯H contacts make the largest contribution to the Hirshfeld surface, accounting for 42.9%, as expected from the high proportion of hydrogen atoms in the organic cation and the importance of van der Waals interactions in the crystal packing.

The H⋯C/C⋯H contacts are also significant, contributing 34.9%, and they correspond to C-H⋯π interactions involving the aromatic rings. The H⋯N/N⋯H and H⋯S/S⋯H contacts contribute 10.7% and 6.4%, respectively, reflecting the presence of classical and non-classical hydrogen bonds involving the thiocyanate anion. In addition, the C⋯S/S⋯C contacts represent 1.4%, while the C⋯C contacts account for 1.5% of the surface.

The remaining intermolecular contacts are only minor, confirming that the supramolecular arrangement is governed primarily by hydrogen bonding, van der Waals interactions and aromatic contacts.

5. Database survey

A search of the Cambridge Structural Database (CSD, version 6.01, updated to February 2026; Groom *et al.*, 2016) for structures related to the title compound gave 1676 hits for organic, non-polymeric, error-free single-crystal entries containing the 4,5-diarylimidazole framework. The closest neutral analogues are the polymorphs of 4,5-diphenyl-1*H*-imidazole [CSD refcodes OCUSUA (Stibrany *et al.*, 2001), OCUSUA01 (Stibrany *et al.*, 2004), OCUSUA02 (Batsanov *et al.*, 2004), OCUSUA03 (Kounavi *et al.*, 2012), OCUSUA04 (Rheingold, 2013)], together with related derivatives such as DPDMTH (King & Sengier, 1978), FASFAH01 (Fridman *et al.*, 2009), FASFAH02 (Huang, 2016) and FOVNIO (Zhang, 2009). More relevant to the present structure are the imidazolium salts GETDIT (Braddock *et al.*, 2006) and PASBEQ (Kaftory *et al.*, 1998), which demonstrate that protonated diarylimidazolium species are known, although no thiocyanate salt of a 4,5-biarylimidazolium cation corresponding to the title compound was identified.

6. Synthesis and crystallization

An equimolar aqueous solution of 4,5-biphenylimidazolium and potassium thiocyanate was prepared in 10 ml of water at room temperature. The reaction mixture was stirred and heated at 343 K for 10 min, then left to evaporate slowly at room temperature. After a few weeks, colourless to white transparent single crystals of the title salt suitable for X-ray diffraction were obtained.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were placed in calculated positions and refined using a riding model, with N—H = 0.86 Å and C—H = 0.93 Å with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier) in all cases.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{13}N_2^+\cdot SCN^-$
M_r	279.35
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, b, c (Å)	6.5328 (3), 12.0855 (5), 18.0627 (8)
V (Å^3)	1426.09 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.22
Crystal size (mm)	0.20 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan *CrysAlis PRO*; Agilent, 2014).
$T_{\rm min}$, $T_{\rm max}$	0.660, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8189, 2428, 2395
$R_{\rm int}$	0.018
$(\sin \theta/\lambda)_{\rm max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.084, 0.92
No. of reflections	2428
No. of parameters	169
No. of restraints	72
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.23, −0.18
Absolute structure	Flack x determined using 919 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.08 (3)

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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References

Agilent (2014). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, England.
Batsanov, A. S., Howard, J. A. K., Martinez, H. & Au-Alvarez, O. (2004). CSD Communication (refcode OCUSUA02). CCDC, Cambridge, England.
Bensegueni, M. A., Cherouana, A., Bendjeddou, L., Lecomte, C. & Dahaoui, S. (2009). *Acta Cryst.* C**65**, o607–o611.
Bensegueni, M. A., Cherouana, A. & Dahaoui, S. (2015). *Acta Cryst.* C**71**, 222–228.
Bensegueni, M. A., Cherouana, A., Dahaoui, S. & Boudraa, I. (2014). *Acta Cryst.* E**70**, m80–m81.
Bensegueni, M. A., Cherouana, A. & Merazig, H. (2020). *Acta Cryst.* E**76**, 877–883.
Braddock, D. C., Hermitage, S. A., Redmond, J. M. & White, A. J. P. (2006). *Tetrahedron Asymmetry* **17**, 2935–2937.
Bruker (2015). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, S.-S. (2016), *CrystEngComm* **18**, 6543–6565.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.

Fridman, N., Kaftory, M., Eichen, Y. & Speiser, S. (2009). *J. Mol. Struct.* **917**, 101–109.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Huang, X. (2016). CSD Communication (refcode FASFAH02). CCDC, Cambridge, England.

Huang, X.-F., Song, Y.-M., Wang, X.-S., Pang, J., Zuo, J.-L. & Xiong, R.-G. (2006). *J. Organomet. Chem.* **691**, 1065–1074.

Kaftory, M., Taycher, H. & Botoshansky, M. (1998). *J. Chem. Soc. Perkin Trans. 2* pp. 407–412.

Kimura, M., Tsunenaga, M., Koyama, T., Iga, H., Aizawa, R., Tachi, Y. & Naruta, Y. (2002). *ITE Lett. Batteries New Technol. Med.*3, 30–33.

King, G. S. D. & Sengier, L. (1978). *Acta Cryst.* A**34**, S112a.

Kounavi, K. A., Manos, M. J., Moushi, E. E., Kitos, A. A., Papatriantafyllopoulou, C., Tasiopoulos, A. J. & Nastopoulos, V. (2012). *Cryst. Growth Des.* **12**, 429–444.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Rheingold, A. L. (2013). CSD Communication (refcode OCUSUA04). CCDC, Cambridge, England.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Stibrany, R. T., Potenza, J. A. & Schugar, H. J. (2001). CSD Communication (refcode OCUSUA). CCDC, Cambridge, England.

Stibrany, R. T., Schugar, H. J. & Potenza, J. A. (2004). *Acta Cryst.* E**60**, o1182–o1184.

Wüstenberg, R. G., Neudörfl, J.-M. & Schmalz, H.-G. (2023). *Isr. J. Chem.* **63**, e2023000, 1–15.

Zhang, Y. (2009). *Acta Cryst.* E**65**, o1675.

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Synthesis and structure of 4,5-diphenyl-1*H*-imidazol-3-ium thiocyanate

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Computing details

4,5-Diphenyl-1*H*-imidazol-3-ium thiocyanate

Crystal data

$C_{15}H_{13}N_2^+\cdot SCN^-$
$M_r = 279.35$
Orthorhombic, $P2_12_12_1$
$a = 6.5328\ (3)$ Å
$b = 12.0855\ (5)$ Å
$c = 18.0627\ (8)$ Å
$V = 1426.09\ (11)$ Å^3
$Z = 4$
$F(000) = 584$

$D_x = 1.301$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7394 reflections
$\theta = 2.2–27.0°$
$\mu = 0.22$ mm^{-1}
$T = 100$ K
Block, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed X-ray tube
ω and phi scans
Absorption correction: multi-scan CrysAlis PRO; Agilent, 2014).
$T_{\min} = 0.660$, $T_{\max} = 1.000$
8189 measured reflections

2428 independent reflections
2395 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.018$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 2.3°$
$h = -7 \rightarrow 7$
$k = -14 \rightarrow 13$
$l = -20 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.084$
$S = 0.92$
2428 reflections
169 parameters
72 restraints
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 1.2893P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Absolute structure: Flack x determined using 919 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.08 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N2	0.8116 (4)	0.70567 (18)	0.70220 (12)	0.0231 (5)
H2	0.756811	0.770267	0.704618	0.028*
N1	1.0144 (4)	0.56874 (19)	0.72286 (13)	0.0234 (5)
H1	1.113206	0.529875	0.740612	0.028*
C2	0.7439 (4)	0.6191 (2)	0.65825 (14)	0.0199 (6)
C3	0.5656 (4)	0.6301 (2)	0.60863 (15)	0.0215 (6)
C9	0.8718 (4)	0.5323 (2)	0.67190 (15)	0.0209 (6)
C1	0.9748 (5)	0.6726 (2)	0.73990 (15)	0.0249 (6)
H1A	1.049153	0.715774	0.772989	0.030*
C8	0.4006 (4)	0.6957 (2)	0.62873 (17)	0.0256 (6)
H8	0.401379	0.732630	0.673906	0.031*
C7	0.2342 (5)	0.7063 (3)	0.58137 (18)	0.0325 (7)
H7	0.123673	0.750352	0.594930	0.039*
C10	0.8736 (3)	0.41895 (12)	0.64286 (11)	0.0242 (6)
C11.	0.6950 (3)	0.35642 (16)	0.64335 (12)	0.0364 (7)
H11.	0.576452	0.384955	0.664493	0.044*
C12	0.6937 (3)	0.25123 (16)	0.61222 (14)	0.0594 (10)
H12	0.574200	0.209394	0.612546	0.071*
C13	0.8709 (5)	0.20858 (14)	0.58061 (13)	0.0676 (11)
H13	0.869996	0.138202	0.559791	0.081*
C14	1.0495 (4)	0.27111 (18)	0.58013 (12)	0.0605 (10)
H14	1.168045	0.242569	0.558982	0.073*
C15	1.0508 (3)	0.37629 (16)	0.61125 (12)	0.0387 (7)
H15	1.170301	0.418130	0.610928	0.046*
C4	0.5655 (5)	0.5773 (2)	0.53980 (16)	0.0268 (7)
H4	0.677352	0.534978	0.525256	0.032*
C6	0.2324 (5)	0.6516 (3)	0.51417 (18)	0.0342 (8)
H6	0.119540	0.657535	0.483036	0.041*
C5	0.3983 (5)	0.5883 (2)	0.49340 (17)	0.0326 (8)
H5	0.397810	0.552654	0.447776	0.039*
S1	0.66610 (13)	0.50873 (8)	0.86212 (5)	0.0427 (3)
N3	0.3105 (4)	0.4330 (2)	0.79293 (15)	0.0325 (6)
C16	0.4590 (5)	0.4652 (2)	0.82209 (16)	0.0259 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0267 (13)	0.0186 (11)	0.0241 (12)	0.0019 (10)	−0.0020 (11)	−0.0028 (10)
N1	0.0216 (12)	0.0244 (12)	0.0241 (12)	0.0022 (10)	−0.0042 (10)	0.0027 (10)
C2	0.0238 (14)	0.0168 (13)	0.0191 (13)	−0.0014 (11)	0.0009 (11)	0.0006 (10)
C3	0.0241 (14)	0.0153 (13)	0.0253 (15)	−0.0039 (12)	−0.0020 (11)	0.0042 (11)
C9	0.0215 (14)	0.0224 (14)	0.0188 (13)	−0.0028 (11)	−0.0008 (11)	0.0018 (11)
C1	0.0271 (15)	0.0259 (15)	0.0216 (15)	−0.0032 (13)	−0.0031 (12)	−0.0034 (11)
C8	0.0262 (15)	0.0225 (14)	0.0281 (16)	−0.0019 (12)	0.0033 (12)	0.0034 (12)
C7	0.0231 (15)	0.0324 (17)	0.0420 (18)	0.0015 (13)	−0.0003 (14)	0.0128 (14)

C10	0.0369 (14)	0.0180 (12)	0.0177 (13)	0.0048 (10)	−0.0048 (11)	0.0030 (11)
C11.	0.0415 (16)	0.0238 (13)	0.0439 (18)	−0.0009 (12)	−0.0213 (15)	0.0059 (13)
C12	0.093 (3)	0.0228 (15)	0.062 (2)	−0.0045 (16)	−0.053 (2)	0.0034 (14)
C13	0.142 (3)	0.0260 (17)	0.035 (2)	0.0237 (17)	−0.039 (2)	−0.0085 (15)
C14	0.116 (3)	0.0386 (17)	0.0265 (17)	0.0392 (17)	0.004 (2)	0.0023 (14)
C15	0.0556 (18)	0.0327 (14)	0.0278 (16)	0.0181 (14)	0.0119 (14)	0.0102 (12)
C4	0.0367 (17)	0.0175 (14)	0.0261 (15)	0.0018 (13)	−0.0032 (13)	0.0013 (11)
C6	0.0339 (17)	0.0316 (17)	0.0371 (17)	−0.0091 (14)	−0.0174 (15)	0.0155 (15)
C5	0.050 (2)	0.0197 (15)	0.0280 (16)	−0.0076 (14)	−0.0147 (15)	0.0024 (12)
S1	0.0329 (4)	0.0460 (5)	0.0491 (5)	−0.0121 (4)	−0.0116 (4)	0.0055 (4)
N3	0.0307 (14)	0.0248 (13)	0.0421 (15)	−0.0007 (12)	−0.0094 (13)	0.0036 (12)
C16	0.0318 (17)	0.0205 (14)	0.0254 (15)	0.0029 (13)	0.0010 (13)	0.0069 (11)

Geometric parameters (Å, º)

N2—C1	1.326 (4)	C10—C15	1.3900
N2—C2	1.386 (3)	C11.—C12	1.3900
N2—H2	0.8600	C11.—H11.	0.9300
N1—C1	1.319 (4)	C12—C13	1.3900
N1—C9	1.382 (4)	C12—H12	0.9300
N1—H1	0.8600	C13—C14	1.3900
C2—C9	1.363 (4)	C13—H13	0.9300
C2—C3	1.476 (4)	C14—C15	1.3900
C3—C8	1.386 (4)	C14—H14	0.9300
C3—C4	1.397 (4)	C15—H15	0.9300
C9—C10	1.468 (3)	C4—C5	1.383 (4)
C1—H1A	0.9300	C4—H4	0.9300
C8—C7	1.389 (4)	C6—C5	1.379 (5)
C8—H8	0.9300	C6—H6	0.9300
C7—C6	1.382 (5)	C5—H5	0.9300
C7—H7	0.9300	S1—C16	1.622 (3)
C10—C11.	1.3900	N3—C16	1.171 (4)
C1—N2—C2	108.9 (2)	C15—C10—C9	119.98 (17)
C1—N2—H2	125.6	C10—C11.—C12	120.0
C2—N2—H2	125.6	C10—C11.—H11.	120.0
C1—N1—C9	109.0 (2)	C12—C11.—H11.	120.0
C1—N1—H1	125.5	C13—C12—C11.	120.0
C9—N1—H1	125.5	C13—C12—H12	120.0
C9—C2—N2	106.3 (2)	C11.—C12—H12	120.0
C9—C2—C3	131.6 (2)	C12—C13—C14	120.0
N2—C2—C3	122.1 (2)	C12—C13—H13	120.0
C8—C3—C4	119.6 (3)	C14—C13—H13	120.0
C8—C3—C2	120.4 (3)	C13—C14—C15	120.0
C4—C3—C2	120.0 (3)	C13—C14—H14	120.0
C2—C9—N1	106.8 (2)	C15—C14—H14	120.0
C2—C9—C10	131.2 (2)	C14—C15—C10	120.0
N1—C9—C10	122.0 (2)	C14—C15—H15	120.0

N1—C1—N2	108.9 (3)	C10—C15—H15	120.0
N1—C1—H1A	125.5	C5—C4—C3	119.7 (3)
N2—C1—H1A	125.5	C5—C4—H4	120.1
C3—C8—C7	120.0 (3)	C3—C4—H4	120.1
C3—C8—H8	120.0	C5—C6—C7	119.8 (3)
C7—C8—H8	120.0	C5—C6—H6	120.1
C6—C7—C8	120.2 (3)	C7—C6—H6	120.1
C6—C7—H7	119.9	C6—C5—C4	120.6 (3)
C8—C7—H7	119.9	C6—C5—H5	119.7
C11.—C10—C15	120.0	C4—C5—H5	119.7
C11.—C10—C9	119.93 (17)	N3—C16—S1	179.4 (3)

C1—N2—C2—C9	0.7 (3)	C2—C9—C10—C11.	−49.5 (4)
C1—N2—C2—C3	−179.2 (2)	N1—C9—C10—C11.	129.8 (2)
C9—C2—C3—C8	145.7 (3)	C2—C9—C10—C15	127.0 (3)
N2—C2—C3—C8	−34.4 (4)	N1—C9—C10—C15	−53.7 (3)
C9—C2—C3—C4	−36.5 (4)	C15—C10—C11.—C12	0.0
N2—C2—C3—C4	143.4 (3)	C9—C10—C11.—C12	176.5 (2)
N2—C2—C9—N1	−0.6 (3)	C10—C11.—C12—C13	0.0
C3—C2—C9—N1	179.2 (3)	C11.—C12—C13—C14	0.0
N2—C2—C9—C10	178.7 (3)	C12—C13—C14—C15	0.0
C3—C2—C9—C10	−1.4 (5)	C13—C14—C15—C10	0.0
C1—N1—C9—C2	0.4 (3)	C11.—C10—C15—C14	0.0
C1—N1—C9—C10	−179.1 (2)	C9—C10—C15—C14	−176.5 (2)
C9—N1—C1—N2	0.1 (3)	C8—C3—C4—C5	−2.0 (4)
C2—N2—C1—N1	−0.5 (3)	C2—C3—C4—C5	−179.7 (2)
C4—C3—C8—C7	1.7 (4)	C8—C7—C6—C5	−1.4 (5)
C2—C3—C8—C7	179.5 (3)	C7—C6—C5—C4	1.2 (5)
C3—C8—C7—C6	0.0 (4)	C3—C4—C5—C6	0.5 (4)

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the N1/C1/N2/C2/C9, C3–C8 and C10–C15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.86	1.98	2.835 (4)	171
N2—H2···N3^{ii}	0.86	2.02	2.862 (3)	168
C12—H12···S1^{iii}	0.93	2.93	3.785 (2)	155
C1—H1*A*···*Cg*3^{iv}	0.93	2.45	3.330 (3)	158
C6—H6···*Cg*2^{v}	0.93	2.93	3.581 (4)	128
C7—H7···*Cg*1^{vi}	0.93	2.91	3.297 (4)	106

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, *y*+1/2, −*z*+3/2; (iii) −*x*+1, *y*−1/2, −*z*+3/2; (iv) −*x*+2, *y*+1/2, −*z*+3/2; (v) *x*−1/2, −*y*+3/2, −*z*+1; (vi) *x*−1, *y*, *z*.