

Received 5 March 2019

Accepted 15 April 2019

Edited by M. Zeller, Purdue University, USA

**Keywords:** crystal structure; imidazole; nagelamide; azide; amide.**CCDC references:** 1910313; 1910312**Supporting information:** this article has supporting information at journals.iucr.org/e

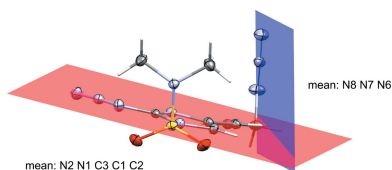
# Crystal structures of 4-[(*E*)-3-[(imino- $\lambda^5$ -azanylidene)amino]prop-1-enyl]-*N,N*-dimethylimidazole-1-sulfonamide and 2-[(imino- $\lambda^5$ -azanylidene)amino]-4-[(*E*)-3-[(imino- $\lambda^5$ -azanylidene)amino]prop-1-enyl]-*N,N*-dimethylimidazole-1-sulfonamide

**Lorenzo M. Cruz,<sup>a</sup> Raakiyah Y. Moore,<sup>a</sup> Marcela Torres Gutierrez,<sup>a</sup> Apsara K. Herath,<sup>b</sup> Carl J. Lovely<sup>b</sup> and Muhammed Yousufuddin<sup>a\*</sup>**<sup>a</sup>Life and Health Sciences Department, University of North Texas at Dallas, 7400 University Hills Blvd, Dallas, TX 75241, USA, and <sup>b</sup>Department of Chemistry and Biochemistry, University of Texas at Arlington, 700 Planetarium Pl., Arlington, TX 76019, USA. \*Correspondence e-mail: myousuf@untDallas.edu

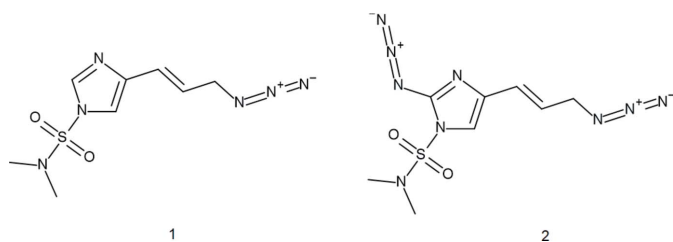
The structures of two azide containing imidazole derivatives are reported. Allylic azides are fairly reactive making them attractive starting compounds to convert into amides. The first,  $C_8H_{12}N_6O_2S$ , contains one azide group with an  $N_\alpha-N_\beta$  distance of 1.229 (2) Å and an  $N_\beta-N_\gamma$  distance of 1.128 (2) Å. The second,  $C_8H_{11}N_9O_2S$ , contains two azide groups with an average  $N_\alpha-N_\beta$  distance of 1.249 (2) Å and an average  $N_\beta-N_\gamma$  distance of 1.132 (2) Å. Each compound contains a bulky protecting group (dimethylaminosulfonyl) which can be easily removed under mildly acidic conditions.

## 1. Chemical context

The efficient synthesis of nagelamide alkaloids (a subfamily of oroidin natural products derived from marine sponges) has garnered interest (Du *et al.*, 2006; Das *et al.*, 2016) since first reported (Endo *et al.*, 2004). Allylic azides (Carlson & Topczewski, 2019) are fairly reactive making them attractive starting compounds to convert into amides. Our group has successfully synthesized a number of azide-containing imidazole derivatives and determined their structures. Many of our strategies have led to the successful synthesis of several nagelamide derivatives (Bhandari *et al.*, 2009; Mukherjee *et al.*, 2010). However, the application of our approaches to several other nagelamide congeners were unsuccessful, leading us to rethink our tactics. Recently, we reported the efficient synthesis of amide compounds from allylic azide-containing imidazoles (Herath *et al.*, 2017). In that report we were also able to show that although the imidazoles contained dimethylaminosulfonyl (DMAS) protecting groups, efficient conversion to amides was still possible. In addition, the free imidazole (lacking the protecting group but still containing azide) underwent selective and rapid conversion to amide without the undesired hydrosulfenylation we observed with protected imidazoles. Here we present the crystal structures of two azide-containing imidazoles, 4-[(*E*)-3-[(imino- $\lambda^5$ -azanylidene)amino]prop-1-enyl]-*N,N*-dimethylimidazole-1-sulfonamide (**1**) and 2-[(imino- $\lambda^5$ -azanylidene)amino]-4-[(*E*)-3-[(imino- $\lambda^5$ -azanylidene)amino]prop-1-enyl]-*N,N*-dimethyl-



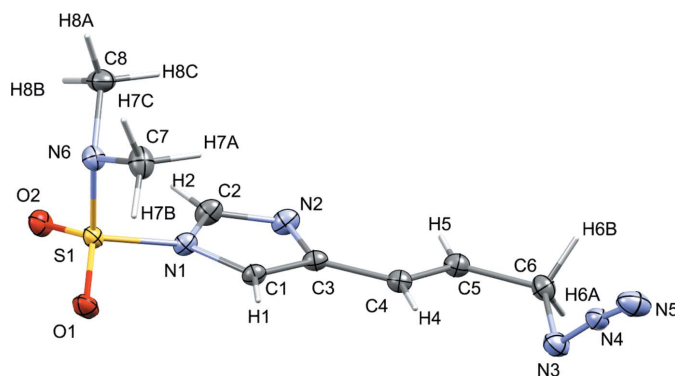
imidazole-1-sulfonamide (**2**). These compounds were synthesized in the previous study but the structures were not reported. Figs. 1 and 2 show displacement ellipsoid plots of **1** and **2**, respectively.



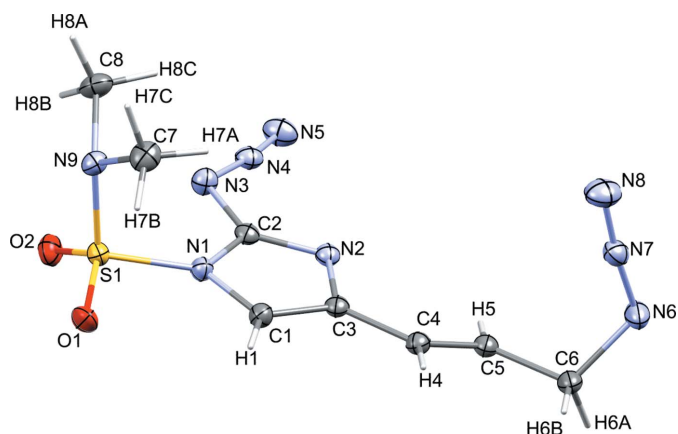
## 2. Structural commentary

Compound **1** contains one allylic azide while compound **2** contains two azide groups, an allylic azide and one azide bound directly to the imidazole ring at C2. The azide group in **1** shows an N3–N4 distance of 1.229 (2) Å and an N4–N5 distance of 1.128 (2) Å. The N3–N4–N5 angle is 172.32 (13)°. The azide groups in **2** show an N3–N4 distance of 1.253 (2) Å, N4–N5 distance of 1.129 (2) Å, N6–N7 distance of 1.239 (2) Å, and N7–N8 distance of 1.134 (2) Å. The N3–N4–N5 angle is 171.58 (15)° and the N6–N7–N8 angle is 173.95 (15)°. All three azide moieties in both compounds show the same general trend of a longer  $N_{\alpha}$ – $N_{\beta}$  distance and shorter  $N_{\beta}$ – $N_{\gamma}$  distance with a quasilinear geometry. This is typical for covalent azides with terminal  $N_{\beta}$ – $N_{\gamma}$  demonstrating more triple-bond character. A previously reported covalent azide occurring in the compound ethyl-2-[(azidocarbonyl)amino]benzoate demonstrated bond lengths  $N_{\alpha}$ – $N_{\beta}$  of 1.264 (2) Å and  $N_{\beta}$ – $N_{\gamma}$  of 1.131 (2) Å and an  $N_{\alpha}$ – $N_{\beta}$ – $N_{\gamma}$  angle of 174.7 (2)° (Yassine *et al.*, 2016).

The torsion angles for the azides and dihedral angles between the azides and imidazole rings for both compounds have been measured. The allylic azide torsion angles between **1** and **2** are quite different. The measured torsion angle for the allylic azide (C5–C6–N3–N4) in **1** was  $-115.21$  (13)° while the related torsion angle (C5–C6–N6–N7) in **2** was  $50.25$  (18)°. **2** contains one azide group bound to the imidazole at C2 and shows a torsion angle N1–C2–N3–N4 of



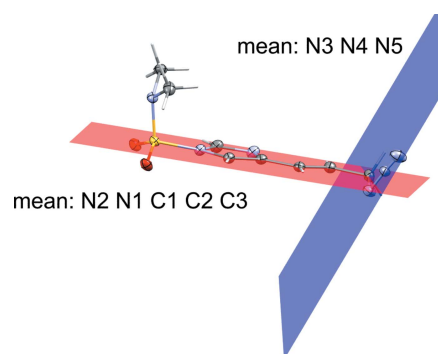
**Figure 1**  
The molecular structure of compound **1**, with atom labels and 50% probability displacement ellipsoids for non-H atoms.



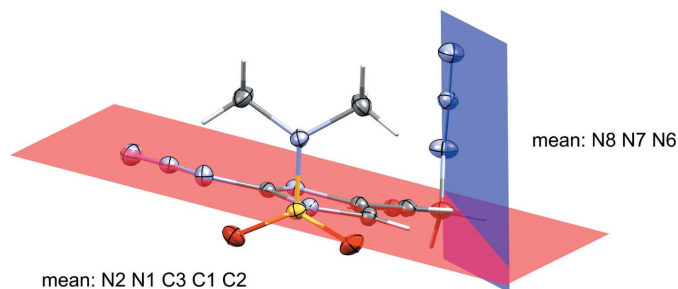
**Figure 2**  
The molecular structure of compound **2**, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

$-174.82$  (11)°. The allylic azides in both compounds exhibit a similar dihedral angle between the azide and the imidazole ring,  $70.3$  (11)° for **1** and  $77.3$  (17)° for **2**. While the imidazole-bound azide in **2** shows a dihedral angle of  $5.0$  (10)°. Indeed, the torsion angle and dihedral angle for this particular azide demonstrate the near planarity between the imidazole and its covalently bound azide. Figs. 3 and 4 show the dihedral planes for **1** and **2**, respectively.

Both title compounds contain a DMAS protecting group. The amine component of this protecting group is  $sp^3$ -hybridized, as validated by the C–N–C bond angles C6–N6–C8 =  $113.86$  (10)° for **1** and C7–N9–C8 =  $113.93$  (12)° for **2**. Both compounds also contain a double bond between C4 and C5.



**Figure 3**  
Dihedral planes between imidazole and allylic azide for compound **1**



**Figure 4**  
Dihedral planes between imidazole and allylic azide for compound **2**

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

| $D-H\cdots A$          | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------|-------|-------------|-------------|---------------|
| $C1-H1\cdots O1^i$     | 0.95  | 2.53        | 3.4487 (18) | 164           |
| $C2-H2\cdots O2^{ii}$  | 0.95  | 2.39        | 3.2861 (18) | 157           |
| $C4-H4\cdots N5^{iii}$ | 0.95  | 2.70        | 3.1920 (17) | 113           |

Symmetry codes: (i)  $-x+2, -y+1, -z+1$ ; (ii)  $-x+2, -y+1, -z+2$ ; (iii)  $x+1, y, z$ .

The measured bond distance is 1.333 (2) Å for **1** and 1.340 (2) Å for **2**.

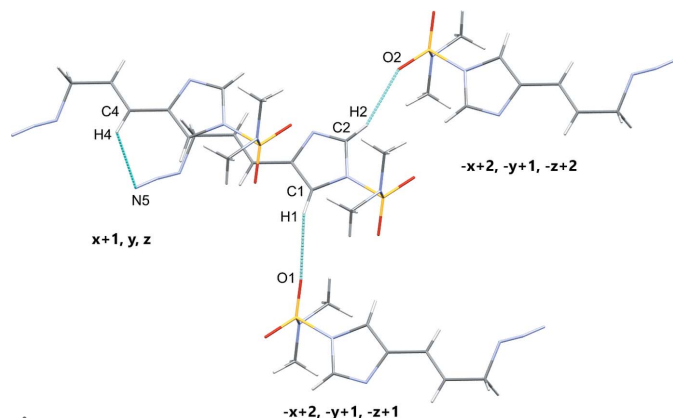
The imidazole ring in **1** is substituted at the N1 and C3 position with no substitution at C2. The N1–C2 distance is 1.378 (2) Å while the N2–C2 distance is 1.301 (2) Å. However, in **2**, the imidazole ring is substituted with an azide group at C2 but this seemingly has no effect on the ring bond distances. The measured bond distances for N1–C2 and N2–C2 in **2** are 1.385 (2) and 1.310 (2) Å, respectively.

There is, however, a significant difference in the measured N1–S1 distance for the two compounds. The imidazole ring is substituted at the N1 position for both compounds with DMAS. The N1–S1 distance for **1** is 1.686 (1) Å and 1.718 (1) Å for **2**. The disparity may be attributed to the presence of azide, which is substituted at the C2 position for **2**.

### 3. Supramolecular features

The title compounds each contain bulky DMAS protecting groups and hydrogen bond distances that influence the molecule packing. Compound **1** shows  $C1-H1\cdots O1^i$  and  $C2-H2\cdots O2^{ii}$  interactions of 2.53 and 2.39 Å, respectively. There is also a  $C4-H4\cdots N5^{iii}$  interaction of 2.70 Å (symmetry codes as in Table 1). Compound **2** demonstrates a  $C7-H7B\cdots O1^i$  interaction of 2.51 Å. There are also  $C6-H6A\cdots N8^{ii}$  and  $C7-H7C\cdots N6^{iii}$  interactions of 2.70 and 2.62 Å, respectively (symmetry codes as in Table 2). Figs. 5 and 6 show the close contacts for **1** and **2**, respectively.

Although both compounds contain aromatic rings, there appears to be no  $\pi$ -stacking present in the crystals of either compound. The stacking appears more staggered, most likely



**Figure 5**  
Close contacts for compound **1**.

**Table 2**  
Hydrogen-bond geometry (Å, °) for **2**.

| $D-H\cdots A$           | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------|-------|-------------|-------------|---------------|
| $C7-H7B\cdots O1^i$     | 0.98  | 2.51        | 3.444 (2)   | 160           |
| $C6-H6A\cdots N8^{ii}$  | 0.99  | 2.70        | 3.337 (2)   | 123           |
| $C7-H7C\cdots N6^{iii}$ | 0.98  | 2.62        | 3.357 (2)   | 132           |

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

due to the presence of bulky DMAS groups on both compounds. However, the staggering in **1** appears more pronounced than in **2**. In other words, the molecules are further apart in **1**. This is most likely due to the larger torsion angle for the azide in **1** than in **2**.

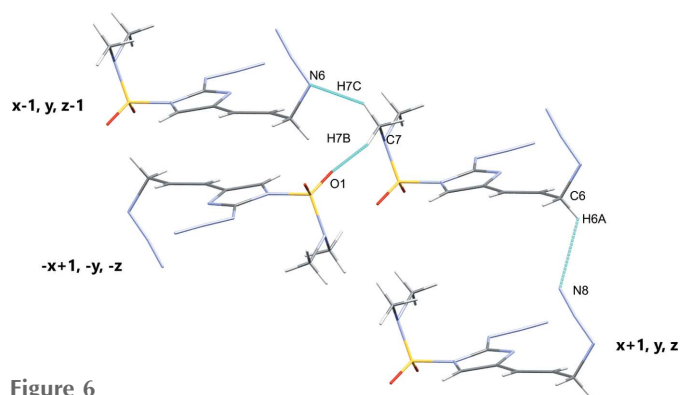
### 4. Database survey

A search of related compounds was conducted in the Cambridge Structural Database (Version 5.38; Groom *et al.*, 2016). One very closely related compound, methyl 3-(1-(dimethylsulfamoyl)-1*H*-imidazol-5-yl)acrylate, was reported (Lovely *et al.*, 2010). This particular compound contains an imidazole with a DMAS protecting group and an allylic ester moiety. The DMAS amine has a C–N–C angle of 114.33 (14)°, showing the same amine hybridization exhibited in **1** and **2**. The C4=C5 double bond distance is measured to be 1.330 (2) Å which is similar to the bond distances in **1** and **2** [1.333 (2) and 1.340 (2) Å respectively].

The crystal structure of a related allylic azide has been reported from our previous study (Herath *et al.*, 2017). This particular compound is a dimerized molecule with two allylic azides.

### 5. Synthesis and crystallization

The syntheses of the title compounds were previously reported by our group (Lovely *et al.*, 2017). As shown in Fig. 7, the parent allylic azide **1** was prepared from the known alcohol starting compound (He *et al.*, 2003) by treatment with diphenylphosphorylazide (DPPA) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) according to the procedure described previously (Thompson *et al.*, 1993). Crystals were acquired by



**Figure 6**  
Close contacts for compound **2**.

**Table 3**  
Experimental details.

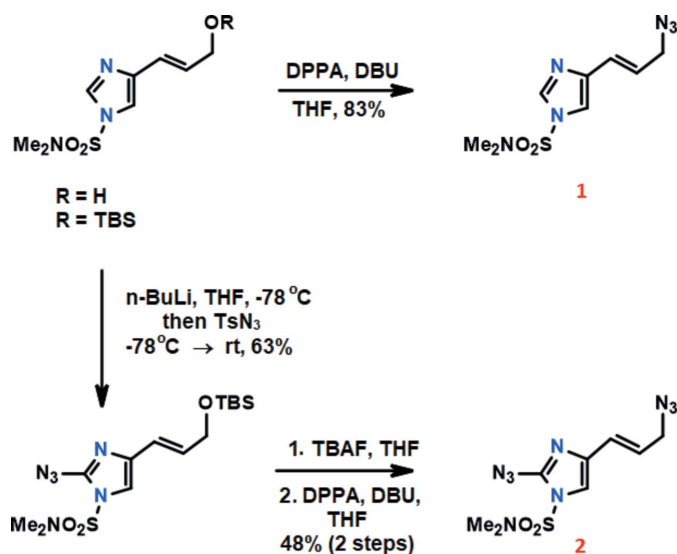
|   | <b>1</b>   | <b>2</b>   |
|---|--|--|
| Crystal data  |  |  |
| Chemical formula  | C <sub>8</sub> H <sub>12</sub> N <sub>6</sub> O <sub>2</sub> S | C <sub>8</sub> H <sub>11</sub> N <sub>9</sub> O <sub>2</sub> S |
| <i>M<sub>r</sub></i>  | 256.30   | 297.32   |
| Crystal system, space group   | Triclinic, <i>P</i> $\bar{1}$                                  | Triclinic, <i>P</i> $\bar{1}$                                  |
| Temperature (K)   | 100  | 100  |
| <i>a</i> , <i>b</i> , <i>c</i> (Å)  | 5.4252 (15), 9.830 (3), 11.137 (3)                             | 6.6151 (18), 9.563 (3), 11.634 (3)                             |
| $\alpha$ , $\beta$ , $\gamma$ (°)   | 74.636 (5), 83.418 (5), 80.255 (5)                             | 108.645 (4), 105.994 (4), 93.828 (4)                           |
| <i>V</i> (Å <sup>3</sup> )  | 563.0 (3)  | 660.6 (3)  |
| <i>Z</i>  | 2  | 2  |
| Radiation type  | Mo <i>K</i> $\alpha$   | Mo <i>K</i> $\alpha$   |
| $\mu$ (mm <sup>-1</sup> )   | 0.29   | 0.26   |
| Crystal size (mm)   | 0.25 × 0.20 × 0.05   | 0.80 × 0.28 × 0.08   |
| Data collection   |  |  |
| Diffractometer  | Bruker D8 Quest  | Bruker D8 Quest  |
| Absorption correction   | Multi-scan ( <i>SADABS</i> ; Bruker, 2016)                     | Multi-scan ( <i>SADABS</i> ; Bruker, 2016)                     |
| <i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>   | 0.616, 0.746   | 0.634, 0.747   |
| No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections                             | 9314, 4292, 3477   | 11030, 5171, 4051  |
| <i>R<sub>int</sub></i>  | 0.033  | 0.030  |
| ( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )   | 0.774  | 0.780  |
| Refinement  |  |  |
| <i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i> | 0.039, 0.104, 1.01   | 0.043, 0.109, 1.07   |
| No. of reflections  | 4292   | 5171   |
| No. of parameters   | 157  | 184  |
| H-atom treatment  | H-atom parameters constrained                                  | H-atom parameters constrained                                  |
| $\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )  | 0.42, -0.48  | 0.46, -0.60  |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2017* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2008) and *SHELXTL* (Sheldrick, 2008).

dissolving title compounds in ethanol with heating and slowly cooling in a freezer. Crystals appeared after about 1 week.

## 6. Refinement

Crystal data, data collection and structure refinement details for **1** and **2** are summarized in Table 3. Refinement for both



**Figure 7**  
Synthetic scheme for both compounds. The title compounds are highlighted in red.

compounds were routine. H atoms were positioned geometrically (C–H = 0.95–0.98 Å) and allowed to ride on their parent atoms, with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C) for methyl H and 1.2*U*<sub>eq</sub>(C) for other H atoms.

## Acknowledgements

The authors thank the Center for Nanostructured Materials at the University of Texas at Arlington for the use of their diffractometer.

## Funding information

Funding for this research was provided by: Robert Welch Foundation (grant No. Y-1362).

## References

- Bhandari, M. R., Sivappa, R. & Lovely, C. J. (2009). *Org. Lett.* **11**, 1535–1538.
- Bruker (2016). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Carlson, A. S. & Topczewski, J. J. (2019). *Org. Bio. Chem.* In the press. doi: 10.1039/C8OB03178A
- Das, J., Bhandari, M. R. & Lovely, C. J. (2016). *edited by Att-ur-Rahman*, Vol. **50**, 341–371: Elsevier.
- Du, H., He, Y., Rasapalli, S. & Lovely, C. J. (2006). *Synlett*, 965–992.
- Endo, T., Tsuda, M., Okada, T., Mitsunashi, S., Shima, H., Kikuchi, K., Mikami, Y., Fromont, J. & Kobayashi, J. (2004). *J. Nat. Prod.* **67**, 1262–1267.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.

- He, Y., Chen, Y., Wu, H. & Lovely, C. J. (2003). *Org. Lett.* **5**, 3623–3626.
- Herath, A. K., Bhandari, M. R., Gout, D., Yousufuddin, M. & Lovely, C. J. (2017). *Tetrahedron Lett.* **58**, 3913–3918.
- Lovely, C. J., Sivappa, R., Mukherjee, S., Doundoulakis, T., Lima, H. M. & Yousufuddin, M. (2010). *Heterocycles*, **80**, 1353–1358.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- Mukherjee, S., Sivappa, R., Yousufuddin, M. & Lovely, C. J. (2010). *Synlett*, pp. 817–821.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Thompson, A. S., Humphrey, G. R., DeMarco, A. M., Mathre, D. J. & Grabowski, E. J. J. (1993). *J. Org. Chem.* **58**, 5886–5888.
- Yassine, H., Hafid, A., Khouili, M., Mentre, O. & Ketatni, E. M. (2016). *IUCrData*, **1**, x161155.

## supporting information

*Acta Cryst.* (2019). E75, 695-699 [https://doi.org/10.1107/S205698901900519X]

## Crystal structures of 4- $\{(E)-3-[(\text{imino-}\lambda^5\text{-azanylidene)amino}]prop-1-enyl\}$ -*N,N*-dimethylimidazole-1-sulfonamide and 2- $\{(E)-3-[(\text{imino-}\lambda^5\text{-azanylidene)amino}]prop-1-enyl\}$ -*N,N*-dimethylimidazole-1-sulfonamide

**Lorenzo M. Cruz, Raakiyah Y. Moore, Marcela Torres Gutierrez, Apsara K. Herath, Carl J. Lovely and Muhammed Yousufuddin**

### Computing details

For both structures, data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXT2014* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

### 4- $\{(E)-3-[(\text{imino-}\lambda^5\text{-azanylidene)amino}]prop-1-enyl\}$ -*N,N*-dimethylimidazole-1-sulfonamide (compound\_1)

#### Crystal data

|                               |   |
|-------------------------------|---|
| $C_8H_{12}N_6O_2S$            | $Z = 2$   |
| $M_r = 256.30$                | $F(000) = 268$  |
| Triclinic, $P\bar{1}$         | $D_x = 1.512 \text{ Mg m}^{-3}$                         |
| $a = 5.4252 (15) \text{ \AA}$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $b = 9.830 (3) \text{ \AA}$   | Cell parameters from 4940 reflections                   |
| $c = 11.137 (3) \text{ \AA}$  | $\theta = 3.2\text{--}33.3^\circ$                       |
| $\alpha = 74.636 (5)^\circ$   | $\mu = 0.29 \text{ mm}^{-1}$                            |
| $\beta = 83.418 (5)^\circ$    | $T = 100 \text{ K}$                                     |
| $\gamma = 80.255 (5)^\circ$   | Prism, colourless                                       |
| $V = 563.0 (3) \text{ \AA}^3$ | $0.25 \times 0.20 \times 0.05 \text{ mm}$               |

#### Data collection

|  |  |
|--|--|
| Bruker D8 Quest diffractometer                           | 4292 independent reflections   |
| $\varphi$ and $\omega$ scans                             | 3477 reflections with $I > 2\sigma(I)$                                 |
| Absorption correction: multi-scan (SADABS; Bruker, 2016) | $R_{\text{int}} = 0.033$   |
| $T_{\text{min}} = 0.616$ , $T_{\text{max}} = 0.746$      | $\theta_{\text{max}} = 33.4^\circ$ , $\theta_{\text{min}} = 3.2^\circ$ |
| 9314 measured reflections                                | $h = -8 \rightarrow 8$   |
|  | $k = -15 \rightarrow 15$   |
|  | $l = -17 \rightarrow 17$   |

#### Refinement

|                                 |                  |
|---------------------------------|------------------|
| Refinement on $F^2$             | $S = 1.01$       |
| Least-squares matrix: full      | 4292 reflections |
| $R[F^2 > 2\sigma(F^2)] = 0.039$ | 157 parameters   |
| $wR(F^2) = 0.104$               | 0 restraints     |

Primary atom site location: structure-invariant  
direct methods

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.2224P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.48 \text{ e } \text{\AA}^{-3}$$

Extinction correction: SHELXL2017

(Sheldrick, 2015b),

$$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.035 (6)

### 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 ( $\text{\AA}^2$ )

|     | <i>x</i>     | <i>y</i>      | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|--------------|----------------------------------|
| S1  | 1.02066 (5)  | 0.56887 (3)   | 0.72049 (3)  | 0.01267 (8)                      |
| O1  | 1.14077 (17) | 0.54225 (11)  | 0.60703 (8)  | 0.01878 (19)                     |
| O2  | 1.15939 (17) | 0.56915 (10)  | 0.82106 (8)  | 0.01797 (18)                     |
| N1  | 0.84664 (19) | 0.43637 (11)  | 0.77979 (9)  | 0.01388 (19)                     |
| N2  | 0.6248 (2)   | 0.28893 (12)  | 0.91880 (10) | 0.0177 (2)                       |
| N3  | 0.1658 (2)   | -0.00361 (13) | 0.71066 (11) | 0.0199 (2)                       |
| N4  | -0.0161 (2)  | 0.04337 (11)  | 0.64781 (10) | 0.0164 (2)                       |
| N5  | -0.1668 (2)  | 0.08138 (15)  | 0.57975 (11) | 0.0256 (3)                       |
| N6  | 0.82889 (19) | 0.71510 (11)  | 0.68919 (10) | 0.01508 (19)                     |
| C1  | 0.7216 (2)   | 0.37309 (13)  | 0.71178 (11) | 0.0140 (2)                       |
| H1  | 0.728564     | 0.389191      | 0.623584     | 0.017*                           |
| C2  | 0.7775 (3)   | 0.38185 (14)  | 0.90406 (11) | 0.0176 (2)                       |
| H2  | 0.834333     | 0.408815      | 0.970797     | 0.021*                           |
| C3  | 0.5864 (2)   | 0.28275 (13)  | 0.79888 (11) | 0.0139 (2)                       |
| C4  | 0.4234 (2)   | 0.19129 (12)  | 0.77555 (11) | 0.0144 (2)                       |
| H4  | 0.407866     | 0.192306      | 0.691209     | 0.017*                           |
| C5  | 0.2939 (2)   | 0.10591 (13)  | 0.86438 (11) | 0.0160 (2)                       |
| H5  | 0.306699     | 0.106802      | 0.948514     | 0.019*                           |
| C6  | 0.1298 (2)   | 0.00877 (14)  | 0.84143 (12) | 0.0174 (2)                       |
| H6A | 0.168435     | -0.086933     | 0.898507     | 0.021*                           |
| H6B | -0.047919    | 0.045775      | 0.860031     | 0.021*                           |
| C7  | 0.6774 (3)   | 0.73822 (15)  | 0.58222 (13) | 0.0211 (3)                       |
| H7A | 0.536984     | 0.683286      | 0.607359     | 0.032*                           |
| H7B | 0.781837     | 0.706956      | 0.513923     | 0.032*                           |
| H7C | 0.612380     | 0.839831      | 0.554136     | 0.032*                           |
| C8  | 0.6881 (3)   | 0.75732 (15)  | 0.79801 (13) | 0.0211 (3)                       |
| H8A | 0.611434     | 0.857329      | 0.772839     | 0.032*                           |
| H8B | 0.802632     | 0.745666      | 0.863140     | 0.032*                           |
| H8C | 0.556684     | 0.697062      | 0.830419     | 0.032*                           |

*Atomic displacement parameters (Å<sup>2</sup>)*

|    | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$      |
|----|--------------|--------------|--------------|--------------|--------------|---------------|
| S1 | 0.01100 (13) | 0.01655 (14) | 0.01073 (13) | -0.00187 (9) | -0.00111 (9) | -0.00383 (10) |
| O1 | 0.0157 (4)   | 0.0266 (5)   | 0.0153 (4)   | -0.0035 (3)  | 0.0026 (3)   | -0.0087 (4)   |
| O2 | 0.0151 (4)   | 0.0247 (5)   | 0.0155 (4)   | -0.0014 (3)  | -0.0055 (3)  | -0.0066 (3)   |
| N1 | 0.0176 (5)   | 0.0138 (4)   | 0.0102 (4)   | -0.0028 (4)  | -0.0014 (3)  | -0.0025 (3)   |
| N2 | 0.0248 (5)   | 0.0166 (5)   | 0.0110 (4)   | -0.0035 (4)  | -0.0011 (4)  | -0.0023 (4)   |
| N3 | 0.0150 (5)   | 0.0256 (6)   | 0.0204 (5)   | -0.0007 (4)  | -0.0020 (4)  | -0.0091 (4)   |
| N4 | 0.0163 (5)   | 0.0170 (5)   | 0.0164 (5)   | -0.0033 (4)  | 0.0022 (4)   | -0.0057 (4)   |
| N5 | 0.0231 (6)   | 0.0337 (7)   | 0.0202 (5)   | 0.0032 (5)   | -0.0023 (4)  | -0.0113 (5)   |
| N6 | 0.0145 (4)   | 0.0154 (5)   | 0.0145 (4)   | -0.0021 (4)  | -0.0026 (4)  | -0.0017 (4)   |
| C1 | 0.0164 (5)   | 0.0154 (5)   | 0.0107 (5)   | -0.0019 (4)  | -0.0014 (4)  | -0.0040 (4)   |
| C2 | 0.0251 (6)   | 0.0176 (5)   | 0.0104 (5)   | -0.0040 (5)  | -0.0021 (4)  | -0.0028 (4)   |
| C3 | 0.0165 (5)   | 0.0133 (5)   | 0.0112 (5)   | -0.0003 (4)  | -0.0009 (4)  | -0.0029 (4)   |
| C4 | 0.0151 (5)   | 0.0145 (5)   | 0.0127 (5)   | -0.0005 (4)  | -0.0012 (4)  | -0.0027 (4)   |
| C5 | 0.0171 (5)   | 0.0174 (5)   | 0.0129 (5)   | -0.0014 (4)  | -0.0012 (4)  | -0.0032 (4)   |
| C6 | 0.0166 (5)   | 0.0190 (5)   | 0.0154 (5)   | -0.0035 (4)  | -0.0003 (4)  | -0.0020 (4)   |
| C7 | 0.0201 (6)   | 0.0213 (6)   | 0.0200 (6)   | -0.0045 (5)  | -0.0075 (5)  | 0.0014 (5)    |
| C8 | 0.0207 (6)   | 0.0191 (6)   | 0.0231 (6)   | 0.0008 (5)   | 0.0013 (5)   | -0.0079 (5)   |

*Geometric parameters (Å, °)*

|          |             |           |             |
|----------|-------------|-----------|-------------|
| S1—O2    | 1.4200 (9)  | C2—H2     | 0.9500      |
| S1—O1    | 1.4209 (10) | C3—C4     | 1.4505 (17) |
| S1—N6    | 1.6067 (11) | C4—C5     | 1.3332 (17) |
| S1—N1    | 1.6858 (11) | C4—H4     | 0.9500      |
| N1—C2    | 1.3783 (15) | C5—C6     | 1.4963 (18) |
| N1—C1    | 1.3896 (15) | C5—H5     | 0.9500      |
| N2—C2    | 1.3012 (17) | C6—H6A    | 0.9900      |
| N2—C3    | 1.3934 (15) | C6—H6B    | 0.9900      |
| N3—N4    | 1.2288 (15) | C7—H7A    | 0.9800      |
| N3—C6    | 1.4814 (17) | C7—H7B    | 0.9800      |
| N4—N5    | 1.1277 (16) | C7—H7C    | 0.9800      |
| N6—C7    | 1.4711 (16) | C8—H8A    | 0.9800      |
| N6—C8    | 1.4736 (17) | C8—H8B    | 0.9800      |
| C1—C3    | 1.3668 (16) | C8—H8C    | 0.9800      |
| C1—H1    | 0.9500      |           |             |
| O2—S1—O1 | 121.78 (6)  | C5—C4—C3  | 124.48 (11) |
| O2—S1—N6 | 108.51 (6)  | C5—C4—H4  | 117.8       |
| O1—S1—N6 | 108.95 (6)  | C3—C4—H4  | 117.8       |
| O2—S1—N1 | 104.30 (6)  | C4—C5—C6  | 124.87 (11) |
| O1—S1—N1 | 105.35 (5)  | C4—C5—H5  | 117.6       |
| N6—S1—N1 | 106.96 (6)  | C6—C5—H5  | 117.6       |
| C2—N1—C1 | 106.84 (10) | N3—C6—C5  | 111.73 (10) |
| C2—N1—S1 | 126.59 (9)  | N3—C6—H6A | 109.3       |
| C1—N1—S1 | 126.18 (8)  | C5—C6—H6A | 109.3       |



|          |             |            |       |
|----------|-------------|------------|-------|
| C2—N2—C3 | 105.77 (10) | N3—C6—H6B  | 109.3 |
| N4—N3—C6 | 116.05 (11) | C5—C6—H6B  | 109.3 |
| N5—N4—N3 | 172.32 (13) | H6A—C6—H6B | 107.9 |
| C7—N6—C8 | 113.86 (10) | N6—C7—H7A  | 109.5 |
| C7—N6—S1 | 116.58 (9)  | N6—C7—H7B  | 109.5 |
| C8—N6—S1 | 115.49 (9)  | H7A—C7—H7B | 109.5 |
| C3—C1—N1 | 105.29 (10) | N6—C7—H7C  | 109.5 |
| C3—C1—H1 | 127.4       | H7A—C7—H7C | 109.5 |
| N1—C1—H1 | 127.4       | H7B—C7—H7C | 109.5 |
| N2—C2—N1 | 111.73 (11) | N6—C8—H8A  | 109.5 |
| N2—C2—H2 | 124.1       | N6—C8—H8B  | 109.5 |
| N1—C2—H2 | 124.1       | H8A—C8—H8B | 109.5 |
| C1—C3—N2 | 110.36 (11) | N6—C8—H8C  | 109.5 |
| C1—C3—C4 | 127.00 (11) | H8A—C8—H8C | 109.5 |
| N2—C3—C4 | 122.65 (11) | H8B—C8—H8C | 109.5 |

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

| <i>D</i> —H $\cdots$ <i>A</i>    | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C1—H1 $\cdots$ O1 <sup>i</sup>   | 0.95        | 2.53                | 3.4487 (18)                | 164                           |
| C2—H2 $\cdots$ O2 <sup>ii</sup>  | 0.95        | 2.39                | 3.2861 (18)                | 157                           |
| C4—H4 $\cdots$ N5 <sup>iii</sup> | 0.95        | 2.70                | 3.1920 (17)                | 113                           |

Symmetry codes: (i)  $-x+2, -y+1, -z+1$ ; (ii)  $-x+2, -y+1, -z+2$ ; (iii)  $x+1, y, z$ .

**2-[(Imino- $\lambda^5$ -azanylidene)amino]-4-[(*E*)-3-[(imino- $\lambda^5$ -azanylidene)amino]prop-1-enyl]-*N,N*-dimethylimidazole-1-sulfonamide (compound\_2)**

*Crystal data*

$\text{C}_8\text{H}_{11}\text{N}_9\text{O}_2\text{S}$   
 $M_r = 297.32$   
 Triclinic,  $P\bar{1}$   
 $a = 6.6151$  (18)  $\text{\AA}$   
 $b = 9.563$  (3)  $\text{\AA}$   
 $c = 11.634$  (3)  $\text{\AA}$   
 $\alpha = 108.645$  (4) $^\circ$   
 $\beta = 105.994$  (4) $^\circ$   
 $\gamma = 93.828$  (4) $^\circ$   
 $V = 660.6$  (3)  $\text{\AA}^3$

$Z = 2$   
 $F(000) = 308$   
 $D_x = 1.495$   $\text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$   $\text{\AA}$   
 Cell parameters from 5257 reflections  
 $\theta = 3.2\text{--}33.6^\circ$   
 $\mu = 0.26$   $\text{mm}^{-1}$   
 $T = 100$  K  
 Needle, colourless  
 $0.80 \times 0.28 \times 0.08$  mm

*Data collection*

Bruker D8 Quest  
 diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2016)  
 $T_{\min} = 0.634$ ,  $T_{\max} = 0.747$   
 11030 measured reflections

5171 independent reflections  
 4051 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$   
 $\theta_{\max} = 33.7^\circ$ ,  $\theta_{\min} = 3.2^\circ$   
 $h = -10 \rightarrow 10$   
 $k = -14 \rightarrow 14$   
 $l = -17 \rightarrow 18$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.109$

$S = 1.07$

5171 reflections

184 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.3565P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$

Extinction correction: SHELXL2017  
(Sheldrick, 2015b),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.022 (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 ( $\text{\AA}^2$ )

|     | <i>x</i>     | <i>y</i>     | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| S1  | 0.58817 (5)  | 0.32361 (4)  | 0.11881 (3)  | 0.01478 (8)                      |
| O1  | 0.65163 (17) | 0.18829 (12) | 0.05384 (10) | 0.0219 (2)                       |
| O2  | 0.66446 (17) | 0.46415 (12) | 0.11471 (10) | 0.0215 (2)                       |
| N1  | 0.68124 (18) | 0.33810 (13) | 0.27604 (10) | 0.0146 (2)                       |
| N2  | 0.75962 (17) | 0.42326 (13) | 0.48977 (10) | 0.0144 (2)                       |
| N3  | 0.64496 (19) | 0.59233 (13) | 0.37520 (11) | 0.0174 (2)                       |
| N4  | 0.67946 (18) | 0.69635 (13) | 0.48007 (11) | 0.0164 (2)                       |
| N5  | 0.7040 (2)   | 0.80092 (15) | 0.56596 (13) | 0.0242 (3)                       |
| N6  | 0.8624 (2)   | 0.18310 (17) | 0.83285 (12) | 0.0237 (3)                       |
| N7  | 0.66897 (19) | 0.15149 (14) | 0.77329 (12) | 0.0193 (2)                       |
| N8  | 0.4889 (2)   | 0.12679 (17) | 0.72893 (15) | 0.0287 (3)                       |
| N9  | 0.33102 (18) | 0.29742 (13) | 0.07962 (11) | 0.0156 (2)                       |
| C1  | 0.7358 (2)   | 0.21797 (15) | 0.31603 (13) | 0.0156 (2)                       |
| H1  | 0.738643     | 0.119381     | 0.263572     | 0.019*                           |
| C2  | 0.69706 (19) | 0.45659 (15) | 0.38610 (12) | 0.0139 (2)                       |
| C3  | 0.78417 (19) | 0.27227 (15) | 0.44638 (12) | 0.0144 (2)                       |
| C4  | 0.8525 (2)   | 0.19077 (15) | 0.53300 (12) | 0.0156 (2)                       |
| H4  | 0.836577     | 0.084831     | 0.497346     | 0.019*                           |
| C5  | 0.9364 (2)   | 0.25679 (16) | 0.66005 (13) | 0.0159 (2)                       |
| H5  | 0.954749     | 0.362879     | 0.695491     | 0.019*                           |
| C6  | 1.0028 (2)   | 0.17314 (17) | 0.74931 (13) | 0.0181 (3)                       |
| H6A | 1.152396     | 0.214636     | 0.803867     | 0.022*                           |
| H6B | 0.996255     | 0.066642     | 0.699097     | 0.022*                           |
| C7  | 0.2306 (2)   | 0.15853 (17) | 0.08670 (15) | 0.0221 (3)                       |
| H7A | 0.250179     | 0.171110     | 0.176261     | 0.033*                           |
| H7B | 0.297367     | 0.074636     | 0.048982     | 0.033*                           |
| H7C | 0.077775     | 0.137969     | 0.039540     | 0.033*                           |

|     |            |              |              |            |
|-----|------------|--------------|--------------|------------|
| C8  | 0.2288 (2) | 0.42873 (17) | 0.12339 (15) | 0.0221 (3) |
| H8A | 0.079649   | 0.408488     | 0.069371     | 0.033*     |
| H8B | 0.304630   | 0.516510     | 0.117531     | 0.033*     |
| H8C | 0.234224   | 0.448176     | 0.212252     | 0.033*     |

*Atomic displacement parameters (Å<sup>2</sup>)*

|    | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|----|--------------|--------------|--------------|--------------|--------------|--------------|
| S1 | 0.01499 (14) | 0.01799 (16) | 0.01287 (14) | 0.00388 (11) | 0.00554 (11) | 0.00623 (11) |
| O1 | 0.0251 (5)   | 0.0260 (5)   | 0.0168 (5)   | 0.0108 (4)   | 0.0107 (4)   | 0.0057 (4)   |
| O2 | 0.0222 (5)   | 0.0242 (5)   | 0.0211 (5)   | −0.0001 (4)  | 0.0076 (4)   | 0.0122 (4)   |
| N1 | 0.0157 (5)   | 0.0157 (5)   | 0.0123 (4)   | 0.0037 (4)   | 0.0040 (4)   | 0.0049 (4)   |
| N2 | 0.0120 (4)   | 0.0159 (5)   | 0.0151 (5)   | 0.0010 (4)   | 0.0043 (4)   | 0.0055 (4)   |
| N3 | 0.0198 (5)   | 0.0148 (5)   | 0.0169 (5)   | 0.0027 (4)   | 0.0053 (4)   | 0.0052 (4)   |
| N4 | 0.0130 (5)   | 0.0164 (5)   | 0.0206 (5)   | 0.0021 (4)   | 0.0064 (4)   | 0.0066 (4)   |
| N5 | 0.0221 (6)   | 0.0208 (6)   | 0.0261 (6)   | 0.0026 (5)   | 0.0090 (5)   | 0.0025 (5)   |
| N6 | 0.0176 (5)   | 0.0379 (7)   | 0.0179 (5)   | 0.0039 (5)   | 0.0057 (4)   | 0.0129 (5)   |
| N7 | 0.0188 (5)   | 0.0212 (6)   | 0.0225 (6)   | 0.0048 (4)   | 0.0100 (4)   | 0.0105 (5)   |
| N8 | 0.0185 (6)   | 0.0307 (7)   | 0.0381 (8)   | 0.0026 (5)   | 0.0097 (5)   | 0.0134 (6)   |
| N9 | 0.0139 (5)   | 0.0152 (5)   | 0.0169 (5)   | 0.0026 (4)   | 0.0030 (4)   | 0.0060 (4)   |
| C1 | 0.0154 (5)   | 0.0160 (6)   | 0.0160 (5)   | 0.0034 (4)   | 0.0047 (4)   | 0.0063 (5)   |
| C2 | 0.0106 (5)   | 0.0148 (5)   | 0.0159 (5)   | 0.0004 (4)   | 0.0044 (4)   | 0.0051 (4)   |
| C3 | 0.0107 (5)   | 0.0169 (6)   | 0.0156 (5)   | 0.0015 (4)   | 0.0037 (4)   | 0.0063 (5)   |
| C4 | 0.0131 (5)   | 0.0178 (6)   | 0.0168 (6)   | 0.0032 (4)   | 0.0044 (4)   | 0.0076 (5)   |
| C5 | 0.0132 (5)   | 0.0193 (6)   | 0.0167 (6)   | 0.0031 (4)   | 0.0053 (4)   | 0.0078 (5)   |
| C6 | 0.0141 (5)   | 0.0254 (7)   | 0.0167 (6)   | 0.0050 (5)   | 0.0051 (4)   | 0.0093 (5)   |
| C7 | 0.0192 (6)   | 0.0195 (7)   | 0.0245 (7)   | −0.0017 (5)  | 0.0028 (5)   | 0.0080 (5)   |
| C8 | 0.0180 (6)   | 0.0203 (7)   | 0.0251 (7)   | 0.0074 (5)   | 0.0042 (5)   | 0.0057 (5)   |

*Geometric parameters (Å, °)*

|       |             |        |             |
|-------|-------------|--------|-------------|
| S1—O2 | 1.4237 (11) | C1—C3  | 1.3707 (18) |
| S1—O1 | 1.4297 (11) | C1—H1  | 0.9500      |
| S1—N9 | 1.6146 (12) | C3—C4  | 1.4579 (18) |
| S1—N1 | 1.7177 (12) | C4—C5  | 1.3402 (19) |
| N1—C2 | 1.3846 (17) | C4—H4  | 0.9500      |
| N1—C1 | 1.4039 (17) | C5—C6  | 1.4961 (19) |
| N2—C2 | 1.3099 (17) | C5—H5  | 0.9500      |
| N2—C3 | 1.4058 (18) | C6—H6A | 0.9900      |
| N3—N4 | 1.2531 (16) | C6—H6B | 0.9900      |
| N3—C2 | 1.4002 (18) | C7—H7A | 0.9800      |
| N4—N5 | 1.1291 (17) | C7—H7B | 0.9800      |
| N6—N7 | 1.2389 (17) | C7—H7C | 0.9800      |
| N6—C6 | 1.5053 (18) | C8—H8A | 0.9800      |
| N7—N8 | 1.1342 (18) | C8—H8B | 0.9800      |
| N9—C8 | 1.4792 (18) | C8—H8C | 0.9800      |
| N9—C7 | 1.4814 (19) |        |             |

|          |             |            |             |
|----------|-------------|------------|-------------|
| O2—S1—O1 | 121.70 (7)  | N2—C3—C4   | 122.43 (12) |
| O2—S1—N9 | 109.81 (6)  | C5—C4—C3   | 123.73 (13) |
| O1—S1—N9 | 108.59 (6)  | C5—C4—H4   | 118.1       |
| O2—S1—N1 | 106.16 (6)  | C3—C4—H4   | 118.1       |
| O1—S1—N1 | 102.88 (6)  | C4—C5—C6   | 123.82 (13) |
| N9—S1—N1 | 106.52 (6)  | C4—C5—H5   | 118.1       |
| C2—N1—C1 | 105.71 (11) | C6—C5—H5   | 118.1       |
| C2—N1—S1 | 129.94 (10) | C5—C6—N6   | 111.84 (11) |
| C1—N1—S1 | 124.00 (9)  | C5—C6—H6A  | 109.2       |
| C2—N2—C3 | 104.81 (11) | N6—C6—H6A  | 109.2       |
| N4—N3—C2 | 114.19 (12) | C5—C6—H6B  | 109.2       |
| N5—N4—N3 | 171.58 (15) | N6—C6—H6B  | 109.2       |
| N7—N6—C6 | 113.91 (12) | H6A—C6—H6B | 107.9       |
| N8—N7—N6 | 173.95 (15) | N9—C7—H7A  | 109.5       |
| C8—N9—C7 | 113.93 (12) | N9—C7—H7B  | 109.5       |
| C8—N9—S1 | 117.77 (10) | H7A—C7—H7B | 109.5       |
| C7—N9—S1 | 115.55 (9)  | N9—C7—H7C  | 109.5       |
| C3—C1—N1 | 105.82 (11) | H7A—C7—H7C | 109.5       |
| C3—C1—H1 | 127.1       | H7B—C7—H7C | 109.5       |
| N1—C1—H1 | 127.1       | N9—C8—H8A  | 109.5       |
| N2—C2—N1 | 113.05 (12) | N9—C8—H8B  | 109.5       |
| N2—C2—N3 | 128.30 (12) | H8A—C8—H8B | 109.5       |
| N1—C2—N3 | 118.64 (11) | N9—C8—H8C  | 109.5       |
| C1—C3—N2 | 110.59 (11) | H8A—C8—H8C | 109.5       |
| C1—C3—C4 | 126.98 (13) | H8B—C8—H8C | 109.5       |

*Hydrogen-bond geometry (Å, °)*

| <i>D</i> —H $\cdots$ <i>A</i>     | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C7—H7B $\cdots$ O1 <sup>i</sup>   | 0.98        | 2.51                | 3.444 (2)                  | 160                           |
| C6—H6A $\cdots$ N8 <sup>ii</sup>  | 0.99        | 2.70                | 3.337 (2)                  | 123                           |
| C7—H7C $\cdots$ N6 <sup>iii</sup> | 0.98        | 2.62                | 3.357 (2)                  | 132                           |

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