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# 4-Nitrophenyl *N*-(2-sulfamoylphenyl)-carbamate

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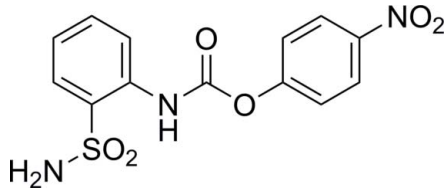
Key indicators: single-crystal X-ray study; $T$ = 180 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.037; $wR$ factor = 0.098; data-to-parameter ratio = 14.7.

In the title molecule, $C_{13}H_{11}N_3O_6S$, the dihedral angle between the benzene rings is 35.52 (8)°. An intramolecular N—H···O hydrogen bond forms an $S$(6) ring. In the crystal, molecules are linked *via* N—H···O hydrogen bonds into chains along [101] incorporating $R_2^2(8)$ and $R_2^2(16)$ rings.

## Related literature

For the synthesis, see: Mallakpour & Rafiee (2007). For hydrogen-bond graph-set motifs, see: Bernstein *et al.* (1995).




## Experimental

### Crystal data

$C_{13}H_{11}N_3O_6S$
$M_r$ = 337.31
Triclinic, $P\overline{1}$
$a$ = 8.2730 (2) Å
$b$ = 8.4881 (2) Å
$c$ = 10.4288 (2) Å
$\alpha$ = 95.178 (1)°
$\beta$ = 103.507 (1)°
$\gamma$ = 94.109 (1)°
$V$ = 705.91 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.27 mm$^{-1}$
$T$ = 180 K
0.27 × 0.27 × 0.12 mm

### Data collection

Nonius KappaCCD diffractometer
21157 measured reflections
3227 independent reflections
2473 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
$S$ = 1.05
3227 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.40 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*1···O3 | 0.802 (19) | 2.02 (2) | 2.6962 (18) | 142.4 (18) |
| N2—H1*N*2···O1$^{i}$ | 0.83 (2) | 2.15 (2) | 2.975 (2) | 175.1 (19) |
| N2—H2*N*2···O4$^{ii}$ | 0.89 (2) | 2.10 (2) | 2.967 (2) | 165 (2) |

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

We are grateful to Dr Sihui Long for providing the help with the crystallization and also in editing this paper. We are grateful to Dr Judith Ann Gallucci for the X-ray crystallographic experiments.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5580).

## References

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# supporting information

*Acta Cryst.* (2013). E**69**, o355 [doi:10.1107/S1600536813003310]

## 4-Nitrophenyl *N*-(2-sulfamoylphenyl)carbamate

**Wenying Yu and Chenglong Li**

### S1. Comment

The title compound (I) is an important intermediate in drug discovery. It was obtained by reacting 2-aminobenzene-sulfonamide with 4-nitrophenyl carbonochloridate through a modified procedure by Mallakpour & Rafiee (2007). The molecular structure of the title compound is shown in Fig. 1. The dihedral angle between the two benzene rings (C1-C6 and C8-C13) is 35.52 (8)°. In the crystal, molecules are linked *via* N—H···O hydrogen bonds (Fig.2) into one-dimensional chains along [101], incorporating $R^2_2(8)$ and $R^2_2(16)$ rings (Bernstein *et al.*, 1995). There is also an intramolecular N—H···O hydrogen bond forming an S(6) ring.

### S2. Experimental

All chemicals were obtained from commercial sources and used directly without further purification. 2-Aminobenzene-sulfonamide (0.72 g, 1 mmol) was dissolved in 10 ml of dry tetrahydrofuran/ dichloromethane (1:1 *v*/*v*), then cooled to 273K. 4-Nitrophenyl carbonochloridate (0.2 g, 1 mmol) was added to the solution in a round-bottom flask, followed by triethylamine (0.14 ml, 1 mmol). The solution was stirred for 1 h at the same temperature and then 2h at room temperature. White solid powder precipitated out (0.307 g, yield: 91%). This was was filtered off, washed with distilled water and dried over anhydrous $Na_2SO_4$. It was characterized by its mass spectrum to be the title compound (I). Colorless plate crystals suitable for X-ray diffraction analysis were grown from a co-solvent system methanol/dichloromethane (1:20 *v*/*v*) solution by slow evaporation at 277K for a week.

### S3. Refinement

H atoms bonded to C atoms were located in difference Fourier maps and were subsequently placed in idealized positions with C—H distances of 0.95Å. They were included in the refinemnt in a riding-motion approxmation with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bonded to N atoms were refined independently with isotropic displacement parameters.

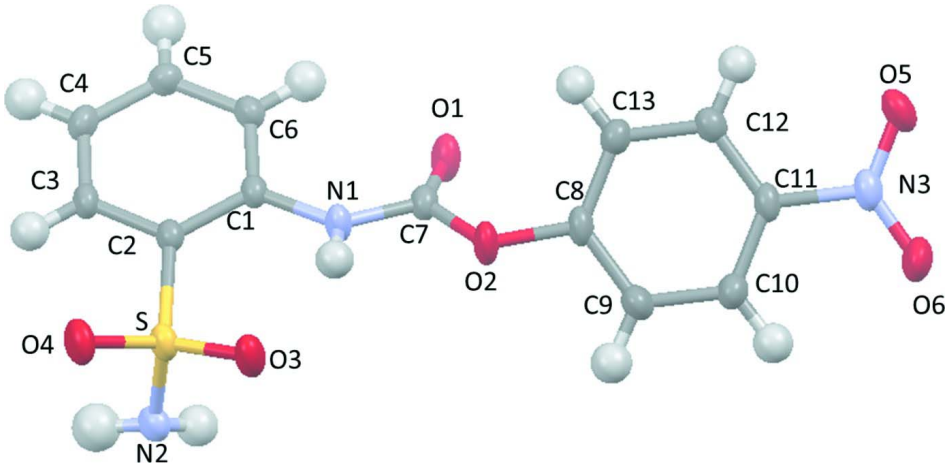


**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

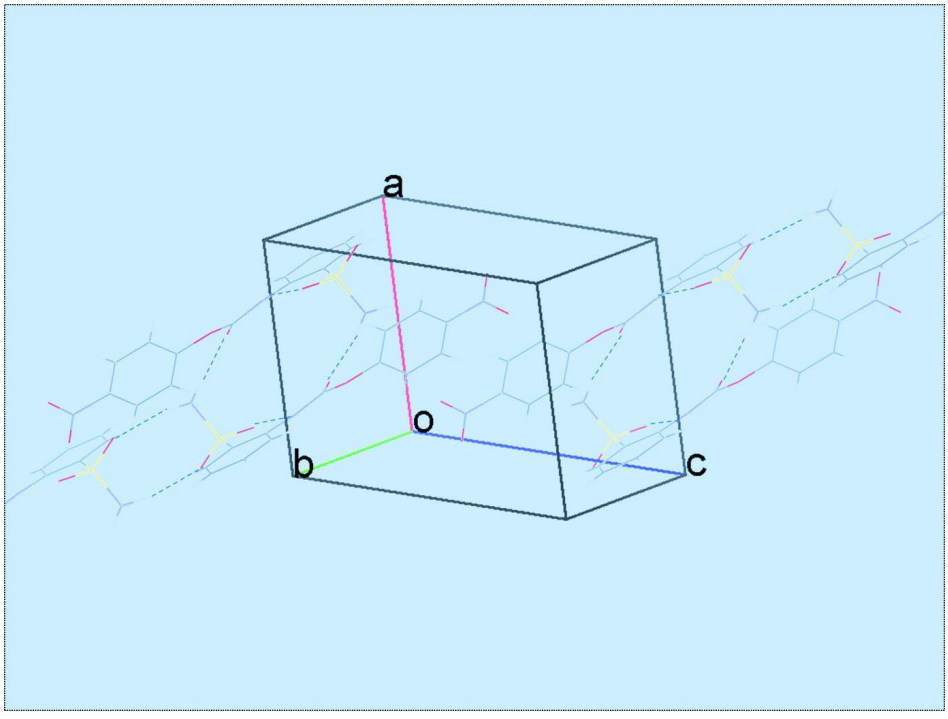


**Figure 2**

Partial crystal packing of the title compound showing the hydrogen bonds as dashed lines.

### 4-Nitrophenyl *N*-(2-sulfamoylphenyl)carbamate

*Crystal data*

$C_{13}H_{11}N_3O_6S$
$M_r = 337.31$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.2730\ (2)$ Å
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$c = 10.4288\ (2)$ Å
$\alpha = 95.178\ (1)°$
$\beta = 103.507\ (1)°$
$\gamma = 94.109\ (1)°$

$V$ = 705.91 (3) Å$^3$
$Z$ = 2
$F$(000) = 348
$D_x$ = 1.587 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 3223 reflections

$\theta$ = 2.0–27.5°
$\mu$ = 0.27 mm$^{-1}$
$T$ = 180 K
Plate, colourless
0.27 × 0.27 × 0.12 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: Enraf Nonius FR590
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
21157 measured reflections

3227 independent reflections
2473 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.4°
$h$ = −10→10
$k$ = −11→11
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
$S$ = 1.05
3227 reflections
220 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.1167P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.40 e Å$^{-3}$

*Special details*

**Experimental**. All work was done at 180 K using an Oxford Cryosystems Cryostream Cooler.
The data collection strategy was set up to measure a hemisphere of reciprocal space with a redundancy factor of 3.6, which means that 90% of these reflections were measured at least 3.6 times. Phi and omega scans with a frame width of 2.0 degrees were used. Data integration was done with *DENZO*, and scaling and merging of the data was done with *SCALEPACK*.

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

**Refinement**. The hydrogen atoms bonded to the nitrogen atoms were located on difference electron density maps, added to the model at these positions and refined isotropically. All three N—H groups are involved in intra and intermolecular hydrogen bonds with the oxygen atoms bonded to the *S* atom and with the oxygen atom of the carbonyl group. The rest of the hydrogen atoms were included in the model at calculated positions using a riding model with U(H) = 1.2*$U_{eq}$(bonded atom).
Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.18448 (19) | 1.06402 (18) | 0.95047 (15) | 0.0243 (3) |
| C2 | 0.09787 (19) | 1.05966 (18) | 0.81639 (15) | 0.0231 (3) |

| | | | | |
|---|---|---|---|---|
| C3 | 0.0295 (2) | 1.19437 (19) | 0.76876 (16) | 0.0283 (4) |
| H3 | −0.0294 | 1.1901 | 0.6785 | 0.034* |
| C4 | 0.0464 (2) | 1.3342 (2) | 0.85148 (17) | 0.0333 (4) |
| H4 | −0.0004 | 1.4259 | 0.8186 | 0.04* |
| C5 | 0.1322 (2) | 1.3391 (2) | 0.98272 (17) | 0.0339 (4) |
| H5 | 0.1446 | 1.4352 | 1.0398 | 0.041* |
| C6 | 0.2001 (2) | 1.2067 (2) | 1.03241 (16) | 0.0314 (4) |
| H6 | 0.258 | 1.2127 | 1.1231 | 0.038* |
| C7 | 0.3599 (2) | 0.91756 (19) | 1.11483 (16) | 0.0261 (4) |
| C8 | 0.4744 (2) | 0.71841 (18) | 1.24599 (16) | 0.0257 (4) |
| C9 | 0.5823 (2) | 0.6064 (2) | 1.22946 (17) | 0.0318 (4) |
| H9 | 0.5904 | 0.568 | 1.143 | 0.038* |
| C10 | 0.6788 (2) | 0.5501 (2) | 1.33996 (16) | 0.0304 (4) |
| H10 | 0.754 | 0.4727 | 1.3309 | 0.036* |
| C11 | 0.66298 (19) | 0.60948 (18) | 1.46359 (16) | 0.0246 (3) |
| C12 | 0.5552 (2) | 0.72220 (18) | 1.48113 (16) | 0.0269 (4) |
| H12 | 0.5475 | 0.761 | 1.5676 | 0.032* |
| C13 | 0.4586 (2) | 0.77744 (19) | 1.37010 (16) | 0.0278 (4) |
| H13 | 0.3829 | 0.8544 | 1.379 | 0.033* |
| N1 | 0.24540 (18) | 0.92648 (17) | 1.00104 (14) | 0.0282 (3) |
| H1N1 | 0.211 (2) | 0.845 (2) | 0.9546 (19) | 0.033 (5)* |
| N2 | 0.2259 (2) | 0.92531 (18) | 0.61879 (15) | 0.0294 (3) |
| H1N2 | 0.322 (3) | 0.939 (2) | 0.668 (2) | 0.039 (6)* |
| H2N2 | 0.197 (3) | 0.993 (3) | 0.559 (2) | 0.053 (6)* |
| N3 | 0.76147 (17) | 0.54610 (16) | 1.58042 (13) | 0.0288 (3) |
| O1 | 0.44001 (14) | 1.02495 (13) | 1.19174 (12) | 0.0354 (3) |
| O2 | 0.37252 (14) | 0.75997 (13) | 1.12918 (11) | 0.0314 (3) |
| O3 | 0.11646 (15) | 0.75518 (13) | 0.76379 (11) | 0.0333 (3) |
| O4 | −0.07382 (14) | 0.89165 (14) | 0.60048 (11) | 0.0333 (3) |
| O5 | 0.73699 (16) | 0.58990 (14) | 1.68935 (11) | 0.0365 (3) |
| O6 | 0.86034 (16) | 0.45021 (16) | 1.56352 (13) | 0.0425 (3) |
| S | 0.08224 (5) | 0.89358 (5) | 0.69623 (4) | 0.02568 (13) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0236 (8) | 0.0292 (8) | 0.0209 (8) | 0.0074 (6) | 0.0035 (6) | 0.0071 (6) |
| C2 | 0.0215 (8) | 0.0268 (8) | 0.0206 (8) | 0.0048 (6) | 0.0025 (6) | 0.0049 (6) |
| C3 | 0.0275 (9) | 0.0360 (9) | 0.0221 (8) | 0.0121 (7) | 0.0025 (7) | 0.0089 (7) |
| C4 | 0.0383 (10) | 0.0341 (9) | 0.0305 (9) | 0.0182 (8) | 0.0075 (8) | 0.0093 (7) |
| C5 | 0.0412 (10) | 0.0333 (9) | 0.0279 (9) | 0.0159 (8) | 0.0070 (8) | 0.0007 (7) |
| C6 | 0.0363 (10) | 0.0379 (10) | 0.0199 (8) | 0.0139 (8) | 0.0033 (7) | 0.0035 (7) |
| C7 | 0.0253 (8) | 0.0294 (9) | 0.0239 (8) | 0.0067 (7) | 0.0037 (7) | 0.0077 (7) |
| C8 | 0.0259 (8) | 0.0249 (8) | 0.0236 (8) | 0.0019 (7) | −0.0017 (7) | 0.0091 (7) |
| C9 | 0.0378 (10) | 0.0363 (10) | 0.0220 (8) | 0.0094 (8) | 0.0061 (7) | 0.0054 (7) |
| C10 | 0.0314 (9) | 0.0331 (9) | 0.0282 (9) | 0.0111 (7) | 0.0061 (7) | 0.0077 (7) |
| C11 | 0.0233 (8) | 0.0249 (8) | 0.0231 (8) | 0.0003 (6) | −0.0005 (6) | 0.0083 (6) |
| C12 | 0.0309 (9) | 0.0264 (8) | 0.0221 (8) | 0.0019 (7) | 0.0041 (7) | 0.0028 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13 | 0.0280 (9) | 0.0263 (8) | 0.0291 (9) | 0.0070 (7) | 0.0042 (7) | 0.0058 (7) |
| N1 | 0.0338 (8) | 0.0256 (8) | 0.0213 (7) | 0.0075 (6) | −0.0031 (6) | 0.0041 (6) |
| N2 | 0.0271 (8) | 0.0359 (8) | 0.0218 (7) | 0.0047 (6) | −0.0002 (6) | 0.0005 (6) |
| N3 | 0.0300 (8) | 0.0277 (7) | 0.0254 (8) | 0.0004 (6) | −0.0011 (6) | 0.0082 (6) |
| O1 | 0.0332 (7) | 0.0303 (6) | 0.0346 (7) | 0.0026 (5) | −0.0094 (6) | 0.0073 (5) |
| O2 | 0.0356 (7) | 0.0277 (6) | 0.0251 (6) | 0.0060 (5) | −0.0068 (5) | 0.0080 (5) |
| O3 | 0.0436 (7) | 0.0251 (6) | 0.0262 (6) | 0.0035 (5) | −0.0025 (5) | 0.0055 (5) |
| O4 | 0.0273 (6) | 0.0382 (7) | 0.0276 (6) | −0.0025 (5) | −0.0065 (5) | 0.0071 (5) |
| O5 | 0.0470 (8) | 0.0380 (7) | 0.0210 (6) | 0.0003 (6) | 0.0014 (6) | 0.0053 (5) |
| O6 | 0.0425 (8) | 0.0487 (8) | 0.0364 (7) | 0.0199 (6) | 0.0018 (6) | 0.0135 (6) |
| S | 0.0258 (2) | 0.0270 (2) | 0.0203 (2) | 0.00131 (16) | −0.00231 (16) | 0.00350 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.397 (2) | C9—C10 | 1.385 (2) |
| C1—N1 | 1.402 (2) | C9—H9 | 0.95 |
| C1—C2 | 1.410 (2) | C10—C11 | 1.380 (2) |
| C2—C3 | 1.392 (2) | C10—H10 | 0.95 |
| C2—S | 1.7758 (16) | C11—C12 | 1.382 (2) |
| C3—C4 | 1.381 (2) | C11—N3 | 1.468 (2) |
| C3—H3 | 0.95 | C12—C13 | 1.385 (2) |
| C4—C5 | 1.382 (2) | C12—H12 | 0.95 |
| C4—H4 | 0.95 | C13—H13 | 0.95 |
| C5—C6 | 1.381 (2) | N1—H1N1 | 0.802 (19) |
| C5—H5 | 0.95 | N2—S | 1.6063 (16) |
| C6—H6 | 0.95 | N2—H1N2 | 0.83 (2) |
| C7—O1 | 1.2028 (19) | N2—H2N2 | 0.89 (2) |
| C7—N1 | 1.346 (2) | N3—O6 | 1.2246 (17) |
| C7—O2 | 1.3680 (19) | N3—O5 | 1.2296 (18) |
| C8—C9 | 1.376 (2) | O3—S | 1.4354 (12) |
| C8—C13 | 1.384 (2) | O4—S | 1.4339 (11) |
| C8—O2 | 1.3999 (18) | | |
| | | | |
| C6—C1—N1 | 121.20 (14) | C11—C10—H10 | 120.9 |
| C6—C1—C2 | 118.12 (14) | C9—C10—H10 | 120.9 |
| N1—C1—C2 | 120.60 (14) | C10—C11—C12 | 122.69 (15) |
| C3—C2—C1 | 120.27 (14) | C10—C11—N3 | 118.21 (14) |
| C3—C2—S | 115.83 (12) | C12—C11—N3 | 119.07 (15) |
| C1—C2—S | 123.72 (12) | C11—C12—C13 | 118.70 (15) |
| C4—C3—C2 | 120.66 (15) | C11—C12—H12 | 120.7 |
| C4—C3—H3 | 119.7 | C13—C12—H12 | 120.7 |
| C2—C3—H3 | 119.7 | C8—C13—C12 | 118.75 (15) |
| C3—C4—C5 | 119.19 (15) | C8—C13—H13 | 120.6 |
| C3—C4—H4 | 120.4 | C12—C13—H13 | 120.6 |
| C5—C4—H4 | 120.4 | C7—N1—C1 | 127.37 (15) |
| C6—C5—C4 | 121.18 (16) | C7—N1—H1N1 | 117.1 (14) |
| C6—C5—H5 | 119.4 | C1—N1—H1N1 | 115.5 (14) |
| C4—C5—H5 | 119.4 | S—N2—H1N2 | 113.9 (14) |

| | | | |
|---|---|---|---|
| C5—C6—C1 | 120.58 (15) | S—N2—H2N2 | 111.1 (14) |
| C5—C6—H6 | 119.7 | H1N2—N2—H2N2 | 118 (2) |
| C1—C6—H6 | 119.7 | O6—N3—O5 | 123.82 (14) |
| O1—C7—N1 | 128.09 (15) | O6—N3—C11 | 118.24 (14) |
| O1—C7—O2 | 124.49 (14) | O5—N3—C11 | 117.92 (13) |
| N1—C7—O2 | 107.42 (14) | C7—O2—C8 | 118.65 (12) |
| C9—C8—C13 | 122.16 (14) | O4—S—O3 | 118.58 (7) |
| C9—C8—O2 | 115.74 (14) | O4—S—N2 | 106.39 (8) |
| C13—C8—O2 | 121.93 (14) | O3—S—N2 | 107.65 (8) |
| C8—C9—C10 | 119.44 (15) | O4—S—C2 | 107.69 (7) |
| C8—C9—H9 | 120.3 | O3—S—C2 | 108.65 (7) |
| C10—C9—H9 | 120.3 | N2—S—C2 | 107.39 (8) |
| C11—C10—C9 | 118.26 (15) | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.5 (2) | C11—C12—C13—C8 | −0.4 (2) |
| N1—C1—C2—C3 | 176.32 (15) | O1—C7—N1—C1 | −4.9 (3) |
| C6—C1—C2—S | 174.44 (13) | O2—C7—N1—C1 | 175.73 (15) |
| N1—C1—C2—S | −8.8 (2) | C6—C1—N1—C7 | −19.4 (3) |
| C1—C2—C3—C4 | 0.5 (3) | C2—C1—N1—C7 | 163.86 (16) |
| S—C2—C3—C4 | −174.82 (13) | C10—C11—N3—O6 | 4.1 (2) |
| C2—C3—C4—C5 | −0.1 (3) | C12—C11—N3—O6 | −177.65 (14) |
| C3—C4—C5—C6 | −0.4 (3) | C10—C11—N3—O5 | −174.26 (15) |
| C4—C5—C6—C1 | 0.4 (3) | C12—C11—N3—O5 | 3.9 (2) |
| N1—C1—C6—C5 | −176.73 (16) | O1—C7—O2—C8 | 5.7 (2) |
| C2—C1—C6—C5 | 0.1 (3) | N1—C7—O2—C8 | −174.90 (14) |
| C13—C8—C9—C10 | −0.1 (3) | C9—C8—O2—C7 | −132.47 (16) |
| O2—C8—C9—C10 | −175.35 (15) | C13—C8—O2—C7 | 52.2 (2) |
| C8—C9—C10—C11 | −0.1 (3) | C3—C2—S—O4 | −35.25 (15) |
| C9—C10—C11—C12 | 0.0 (3) | C1—C2—S—O4 | 149.62 (14) |
| C9—C10—C11—N3 | 178.11 (15) | C3—C2—S—O3 | −164.86 (12) |
| C10—C11—C12—C13 | 0.3 (3) | C1—C2—S—O3 | 20.01 (16) |
| N3—C11—C12—C13 | −177.85 (14) | C3—C2—S—N2 | 78.97 (14) |
| C9—C8—C13—C12 | 0.3 (3) | C1—C2—S—N2 | −96.16 (15) |
| O2—C8—C13—C12 | 175.31 (14) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*1···O3 | 0.802 (19) | 2.02 (2) | 2.6962 (18) | 142.4 (18) |
| N1—H1*N*1···S | 0.802 (19) | 2.736 (19) | 3.1283 (14) | 112.2 (15) |
| N2—H1*N*2···O1$^{i}$ | 0.83 (2) | 2.15 (2) | 2.975 (2) | 175.1 (19) |
| N2—H2*N*2···O4$^{ii}$ | 0.89 (2) | 2.10 (2) | 2.967 (2) | 165 (2) |

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+2; (ii) −*x*, −*y*+2, −*z*+1.