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2-(2-Thienylmethyleneamino)isoindoline-1,3-dione

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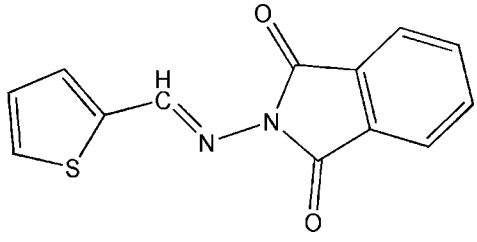
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.130; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound, $C_{13}H_8N_2O_2S$, contains two independent molecules. The thiophene ring is planar [r.m.s. deviation = 0.0015 (5) Å]. The r.m.s. deviation for the isoindoline group is 0.0195 (4) Å. The dihedral angle between the two planes is 12.9 (2)°. The crystal structure is stabilized by weak intermolecular interactions to form a three-dimensional network.

Related literature

For general background, see: Belloni *et al.* (2005); Kahwa *et al.* (1986); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005).



Experimental

Crystal data

$C_{13}H_8N_2O_2S$
M_r = 256.27
Monoclinic, $P2_1/c$
a = 8.4727 (15) Å
b = 21.327 (4) Å
c = 12.942 (2) Å
β = 90.740 (3)°
V = 2338.4 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 294 (2) K
0.26 × 0.22 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.933, T_{max} = 0.963
13313 measured reflections
4790 independent reflections
2978 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.00
4790 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2357).

References

Belloni, M., Kariuki, B. M., Manickam, M., Wilkie, J. & Preece, J. A. (2005). *Cryst. Growth Des.* **5**, 1443–1449.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0). Bruker AXS Inc., Madison, Wisconsin, USA.
Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.
Parashar, R. K., Sharma, R. C., Kumar, A. & Mohan, G. (1988). *Inorg. Chim. Acta*, **151**, 201–208.
Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tynan, E., Jensen, P., Lees, A. C., Moubaraki, B., Murray, K. S. & Kruger, P. E. (2005). *CrystEngComm*, **7**, 90–95.

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supplementary materials

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2-(2-Thienylmethyleneamino)isoindoline-1,3-dione

Z.-L. Jing, M. Yu and X. Chen

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of the active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*,2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands, we report the synthesis and crystal structure of the title compound, (I).

In the molecular structure of the compound (I) (Fig. 1), the geometric parameters are normal. In one molecule of the unit, the thiophen ring (C1—C4/S1) is approximately planar, with a maximum deviation from the mean plane of 0.0015 (5) Å for atom S1, as the isoindoline group (C6—C13/N2) is approximately planar, with a maximum deviation from the mean plane of 0.0195 (4) Å for atom N2. The dihedral angle between these two planes is12.9(1)°. In the other molecule of the unit, the thiophen ring (C14—C17/S2) is approximately planar, with a maximum deviation from the mean plane of 0.0019 (2) Å for atom S2, as the isoindoline group (C19—C26/N4) is approximately planar, with a maximum deviation from the mean plane of 0.0187 (4) Å for atom N4. The dihedral angle between these two planes is14.2(3)°. The molecular structure stabilized by the weak intermolecular interactions to form a three-dimensional network, as illustraed in Fig.2.

Experimental

An anhydrous ethanol solution (50 ml) of thiophene-2-carbaldehyde (1.12 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of *N*-Amino-phthalimide (1.52 g, 10 mmol), and the mixture was stirred at 350 K for 6 h under N_2, whereupon a yellow precipitate appeared. The product was isolated, recrystallized from anhydrous ethanol and then dried *in vacuo* to give pure compound (I) in 79% yield. Yellows single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution.

Refinement

The H atoms were included in calculated positions, with C—H = 0.93 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

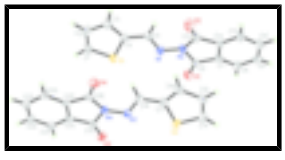


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

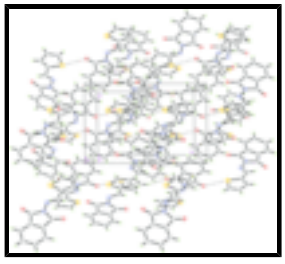


Fig. 2. The crystal packing of (I), viwed down the *b* axis. Hydrogen bonds are indicated by dashed lines.

2-(2-Thienylmethyleneamino)isoindoline-1,3-dione

Crystal data

$C_{13}H_8N_2O_2S$	F_{000} = 1056
M_r = 256.27	D_x = 1.456 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3262 reflections
a = 8.4727 (15) Å	θ = 2.4–23.6º
b = 21.327 (4) Å	μ = 0.27 mm^{-1}
c = 12.942 (2) Å	T = 294 (2) K
β = 90.740 (3)º	Block, yellow
V = 2338.4 (7) Å^3	0.26 × 0.22 × 0.14 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	4790 independent reflections
Radiation source: fine-focus sealed tube	2978 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→10
T_{min} = 0.933, T_{max} = 0.963	k = −26→20
13313 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.130	$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.4001P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001
4790 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}

325 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

Refinement. 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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.31619 (9)	0.53967 (3)	0.74090 (5)	0.0538 (2)
S2	0.32169 (10)	0.27454 (4)	0.82918 (6)	0.0642 (2)
O1	−0.0683 (2)	0.36649 (9)	0.76193 (13)	0.0576 (5)
O2	0.1037 (3)	0.38058 (10)	0.42808 (14)	0.0726 (6)
O3	0.5966 (2)	0.43516 (8)	1.03183 (13)	0.0515 (5)
O4	0.7077 (2)	0.46997 (8)	0.68989 (12)	0.0518 (5)
N1	0.1224 (2)	0.44033 (9)	0.63749 (15)	0.0454 (5)
N2	0.0281 (2)	0.39189 (9)	0.59954 (14)	0.0423 (5)
N3	0.5253 (2)	0.38981 (9)	0.83827 (15)	0.0420 (5)
N4	0.6191 (2)	0.44210 (8)	0.85373 (14)	0.0398 (5)
C1	0.4415 (3)	0.59990 (12)	0.7181 (2)	0.0543 (7)
H1	0.4896	0.6235	0.7700	0.065*
C2	0.4635 (4)	0.60972 (14)	0.6173 (2)	0.0721 (9)
H2	0.5293	0.6408	0.5918	0.087*
C3	0.3771 (4)	0.56820 (13)	0.5535 (2)	0.0646 (8)
H3	0.3788	0.5688	0.4816	0.077*
C4	0.2893 (3)	0.52645 (11)	0.61120 (18)	0.0436 (6)
C5	0.1893 (3)	0.47651 (12)	0.5731 (2)	0.0487 (6)
H5	0.1740	0.4708	0.5024	0.058*
C6	−0.0622 (3)	0.35680 (11)	0.67075 (18)	0.0423 (6)
C7	−0.1402 (3)	0.30689 (11)	0.60781 (18)	0.0412 (6)
C8	−0.2488 (3)	0.26202 (12)	0.6354 (2)	0.0507 (7)
H8	−0.2855	0.2592	0.7026	0.061*
C9	−0.3011 (3)	0.22104 (12)	0.5587 (2)	0.0563 (7)
H9	−0.3761	0.1908	0.5747	0.068*
C10	−0.2443 (3)	0.22424 (13)	0.4595 (2)	0.0592 (7)
H10	−0.2797	0.1956	0.4102	0.071*
C11	−0.1353 (3)	0.26951 (13)	0.4323 (2)	0.0582 (7)
H11	−0.0965	0.2719	0.3656	0.070*
C12	−0.0866 (3)	0.31089 (12)	0.50782 (18)	0.0451 (6)

C13	0.0251 (3)	0.36405 (12)	0.50107 (19)	0.0484 (6)
C14	0.2387 (4)	0.22267 (14)	0.7441 (2)	0.0642 (8)
H14	0.1872	0.1862	0.7642	0.077*
C15	0.2556 (3)	0.23996 (13)	0.6455 (2)	0.0589 (8)
H15	0.2173	0.2170	0.5894	0.071*
C16	0.3380 (3)	0.29693 (13)	0.6365 (2)	0.0530 (7)
H16	0.3597	0.3159	0.5736	0.064*
C17	0.3828 (3)	0.32148 (11)	0.72955 (19)	0.0447 (6)
C18	0.4755 (3)	0.37733 (11)	0.7475 (2)	0.0468 (6)
H18	0.4987	0.4040	0.6929	0.056*
C19	0.6516 (3)	0.46019 (11)	0.95717 (18)	0.0390 (6)
C20	0.7642 (3)	0.51331 (10)	0.94960 (17)	0.0366 (5)
C21	0.8318 (3)	0.54996 (11)	1.02630 (18)	0.0437 (6)
H21	0.8052	0.5448	1.0953	0.052*
C22	0.9408 (3)	0.59478 (12)	0.99646 (19)	0.0475 (6)
H22	0.9880	0.6204	1.0462	0.057*
C23	0.9802 (3)	0.60191 (11)	0.89348 (19)	0.0481 (6)
H23	1.0554	0.6317	0.8757	0.058*
C24	0.9107 (3)	0.56591 (11)	0.81649 (19)	0.0443 (6)
H24	0.9363	0.5713	0.7474	0.053*
C25	0.8019 (3)	0.52176 (10)	0.84651 (17)	0.0370 (5)
C26	0.7089 (3)	0.47684 (11)	0.78229 (18)	0.0388 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0587 (4)	0.0627 (5)	0.0403 (4)	−0.0125 (4)	0.0053 (3)	−0.0081 (3)
S2	0.0822 (6)	0.0567 (5)	0.0536 (4)	−0.0137 (4)	−0.0037 (4)	0.0069 (3)
O1	0.0730 (13)	0.0640 (12)	0.0360 (10)	−0.0058 (10)	0.0066 (9)	−0.0051 (8)
O2	0.0948 (16)	0.0811 (14)	0.0423 (11)	−0.0369 (12)	0.0186 (11)	−0.0133 (10)
O3	0.0634 (12)	0.0519 (11)	0.0392 (10)	−0.0081 (9)	0.0066 (9)	0.0039 (8)
O4	0.0648 (12)	0.0578 (11)	0.0328 (9)	−0.0057 (9)	−0.0019 (8)	−0.0012 (8)
N1	0.0495 (13)	0.0453 (12)	0.0413 (12)	−0.0047 (10)	−0.0006 (10)	−0.0083 (10)
N2	0.0486 (12)	0.0445 (12)	0.0337 (11)	−0.0069 (10)	0.0005 (9)	−0.0068 (9)
N3	0.0439 (12)	0.0366 (11)	0.0454 (12)	0.0000 (9)	−0.0041 (9)	−0.0003 (9)
N4	0.0464 (12)	0.0354 (11)	0.0374 (11)	−0.0027 (9)	0.0002 (9)	−0.0022 (9)
C1	0.0537 (17)	0.0537 (16)	0.0555 (17)	−0.0115 (14)	0.0023 (13)	−0.0168 (13)
C2	0.094 (3)	0.068 (2)	0.0545 (18)	−0.0365 (18)	0.0124 (17)	0.0001 (15)
C3	0.096 (2)	0.0636 (19)	0.0345 (14)	−0.0246 (17)	−0.0010 (14)	−0.0025 (13)
C4	0.0487 (15)	0.0433 (14)	0.0389 (13)	−0.0003 (12)	0.0002 (11)	−0.0045 (11)
C5	0.0578 (17)	0.0480 (15)	0.0401 (14)	−0.0042 (13)	−0.0053 (12)	−0.0059 (12)
C6	0.0448 (15)	0.0441 (14)	0.0381 (14)	0.0050 (12)	0.0009 (11)	−0.0007 (11)
C7	0.0393 (14)	0.0414 (13)	0.0428 (14)	0.0042 (11)	−0.0012 (11)	−0.0007 (11)
C8	0.0492 (16)	0.0478 (16)	0.0553 (16)	0.0005 (13)	0.0077 (13)	0.0052 (13)
C9	0.0492 (17)	0.0403 (15)	0.079 (2)	−0.0060 (13)	0.0023 (15)	0.0010 (14)
C10	0.0607 (18)	0.0518 (17)	0.0649 (19)	−0.0060 (15)	−0.0091 (15)	−0.0127 (14)
C11	0.0662 (19)	0.0585 (18)	0.0500 (16)	−0.0123 (15)	0.0000 (14)	−0.0129 (13)
C12	0.0466 (15)	0.0461 (15)	0.0427 (14)	−0.0027 (12)	0.0002 (12)	−0.0044 (11)

C13	0.0558 (17)	0.0502 (16)	0.0393 (14)	−0.0075 (13)	0.0027 (12)	−0.0048 (12)
C14	0.068 (2)	0.0435 (16)	0.080 (2)	−0.0117 (14)	−0.0046 (17)	−0.0002 (14)
C15	0.0622 (19)	0.0571 (18)	0.0571 (18)	−0.0103 (15)	−0.0056 (14)	−0.0119 (14)
C16	0.0582 (17)	0.0543 (16)	0.0465 (15)	−0.0106 (14)	−0.0013 (13)	−0.0039 (13)
C17	0.0411 (14)	0.0422 (14)	0.0507 (15)	0.0021 (12)	−0.0004 (12)	0.0012 (12)
C18	0.0542 (16)	0.0405 (14)	0.0457 (15)	−0.0039 (12)	−0.0018 (12)	0.0043 (11)
C19	0.0435 (14)	0.0372 (13)	0.0363 (13)	0.0053 (11)	0.0001 (11)	−0.0005 (10)
C20	0.0385 (13)	0.0332 (12)	0.0381 (12)	0.0051 (11)	0.0005 (10)	0.0007 (10)
C21	0.0527 (16)	0.0424 (14)	0.0359 (13)	0.0025 (12)	0.0031 (11)	−0.0011 (11)
C22	0.0543 (16)	0.0416 (14)	0.0463 (15)	−0.0002 (13)	−0.0057 (12)	−0.0048 (12)
C23	0.0492 (16)	0.0412 (14)	0.0540 (16)	−0.0052 (12)	0.0009 (13)	0.0056 (12)
C24	0.0484 (15)	0.0461 (15)	0.0385 (13)	0.0019 (12)	0.0029 (12)	0.0062 (11)
C25	0.0408 (14)	0.0346 (12)	0.0355 (12)	0.0060 (11)	−0.0007 (10)	0.0017 (10)
C26	0.0414 (14)	0.0386 (13)	0.0364 (13)	0.0056 (11)	−0.0022 (11)	0.0022 (11)

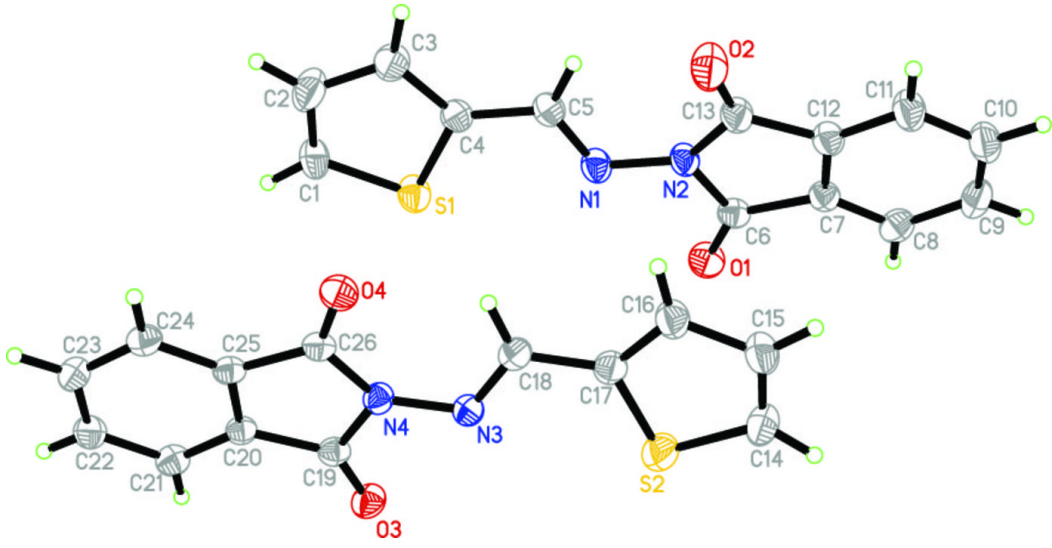
Geometric parameters (Å, °)

S1—C1	1.695 (3)	C8—H8	0.9300
S1—C4	1.715 (2)	C9—C10	1.379 (4)
S2—C14	1.706 (3)	C9—H9	0.9300
S2—C17	1.718 (2)	C10—C11	1.385 (4)
O1—C6	1.200 (3)	C10—H10	0.9300
O2—C13	1.215 (3)	C11—C12	1.376 (3)
O3—C19	1.203 (3)	C11—H11	0.9300
O4—C26	1.205 (3)	C12—C13	1.480 (3)
N1—C5	1.274 (3)	C14—C15	1.338 (4)
N1—N2	1.392 (3)	C14—H14	0.9300
N2—C13	1.406 (3)	C15—C16	1.407 (4)
N2—C6	1.418 (3)	C15—H15	0.9300
N3—C18	1.272 (3)	C16—C17	1.362 (3)
N3—N4	1.383 (3)	C16—H16	0.9300
N4—C26	1.415 (3)	C17—C18	1.444 (3)
N4—C19	1.417 (3)	C18—H18	0.9300
C1—C2	1.337 (3)	C19—C20	1.485 (3)
C1—H1	0.9300	C20—C21	1.382 (3)
C2—C3	1.409 (4)	C20—C25	1.388 (3)
C2—H2	0.9300	C21—C22	1.387 (3)
C3—C4	1.385 (4)	C21—H21	0.9300
C3—H3	0.9300	C22—C23	1.387 (3)
C4—C5	1.443 (3)	C22—H22	0.9300
C5—H5	0.9300	C23—C24	1.384 (3)
C6—C7	1.490 (3)	C23—H23	0.9300
C7—C8	1.377 (3)	C24—C25	1.377 (3)
C7—C12	1.380 (3)	C24—H24	0.9300
C8—C9	1.391 (4)	C25—C26	1.487 (3)
C1—S1—C4	91.71 (12)	C11—C12—C13	129.5 (2)
C14—S2—C17	91.10 (14)	C7—C12—C13	108.7 (2)
C5—N1—N2	118.5 (2)	O2—C13—N2	125.3 (2)
N1—N2—C13	129.58 (19)	O2—C13—C12	128.7 (2)

N1—N2—C6	118.30 (18)	N2—C13—C12	105.9 (2)
C13—N2—C6	111.26 (19)	C15—C14—S2	112.9 (2)
C18—N3—N4	119.1 (2)	C15—C14—H14	123.6
N3—N4—C26	129.87 (19)	S2—C14—H14	123.6
N3—N4—C19	117.42 (18)	C14—C15—C16	112.1 (2)
C26—N4—C19	112.06 (19)	C14—C15—H15	124.0
C2—C1—S1	112.6 (2)	C16—C15—H15	124.0
C2—C1—H1	123.7	C17—C16—C15	113.1 (2)
S1—C1—H1	123.7	C17—C16—H16	123.5
C1—C2—C3	113.3 (3)	C15—C16—H16	123.5
C1—C2—H2	123.4	C16—C17—C18	127.1 (2)
C3—C2—H2	123.4	C16—C17—S2	110.86 (19)
C4—C3—C2	111.5 (2)	C18—C17—S2	121.93 (19)
C4—C3—H3	124.3	N3—C18—C17	119.6 (2)
C2—C3—H3	124.3	N3—C18—H18	120.2
C3—C4—C5	127.4 (2)	C17—C18—H18	120.2
C3—C4—S1	110.90 (19)	O3—C19—N4	124.5 (2)
C5—C4—S1	121.72 (19)	O3—C19—C20	130.3 (2)
N1—C5—C4	119.2 (2)	N4—C19—C20	105.21 (19)
N1—C5—H5	120.4	C21—C20—C25	121.3 (2)
C4—C5—H5	120.4	C21—C20—C19	130.1 (2)
O1—C6—N2	125.3 (2)	C25—C20—C19	108.6 (2)
O1—C6—C7	129.5 (2)	C20—C21—C22	117.4 (2)
N2—C6—C7	105.12 (19)	C20—C21—H21	121.3
C8—C7—C12	121.0 (2)	C22—C21—H21	121.3
C8—C7—C6	130.4 (2)	C23—C22—C21	120.8 (2)
C12—C7—C6	108.6 (2)	C23—C22—H22	119.6
C7—C8—C9	117.4 (2)	C21—C22—H22	119.6
C7—C8—H8	121.3	C24—C23—C22	121.7 (2)
C9—C8—H8	121.3	C24—C23—H23	119.1
C10—C9—C8	121.4 (3)	C22—C23—H23	119.1
C10—C9—H9	119.3	C25—C24—C23	117.2 (2)
C8—C9—H9	119.3	C25—C24—H24	121.4
C9—C10—C11	120.9 (3)	C23—C24—H24	121.4
C9—C10—H10	119.6	C24—C25—C20	121.6 (2)
C11—C10—H10	119.6	C24—C25—C26	129.4 (2)
C12—C11—C10	117.5 (3)	C20—C25—C26	109.1 (2)
C12—C11—H11	121.2	O4—C26—N4	126.0 (2)
C10—C11—H11	121.2	O4—C26—C25	129.1 (2)
C11—C12—C7	121.8 (2)	N4—C26—C25	104.93 (19)
C5—N1—N2—C13	19.7 (4)	C11—C12—C13—N2	178.0 (3)
C5—N1—N2—C6	−172.0 (2)	C7—C12—C13—N2	−2.4 (3)
C18—N3—N4—C26	−19.8 (3)	C17—S2—C14—C15	−0.2 (2)
C18—N3—N4—C19	170.2 (2)	S2—C14—C15—C16	0.0 (3)
C4—S1—C1—C2	−0.4 (3)	C14—C15—C16—C17	0.3 (4)
S1—C1—C2—C3	0.4 (4)	C15—C16—C17—C18	176.6 (2)
C1—C2—C3—C4	−0.2 (4)	C15—C16—C17—S2	−0.5 (3)
C2—C3—C4—C5	−178.6 (3)	C14—S2—C17—C16	0.4 (2)
C2—C3—C4—S1	−0.1 (3)	C14—S2—C17—C18	−176.8 (2)

C1—S1—C4—C3	0.2 (2)	N4—N3—C18—C17	177.5 (2)
C1—S1—C4—C5	178.9 (2)	C16—C17—C18—N3	−170.8 (3)
N2—N1—C5—C4	−179.2 (2)	S2—C17—C18—N3	6.0 (3)
C3—C4—C5—N1	176.7 (3)	N3—N4—C19—O3	−4.0 (3)
S1—C4—C5—N1	−1.8 (4)	C26—N4—C19—O3	−175.7 (2)
N1—N2—C6—O1	2.4 (4)	N3—N4—C19—C20	175.23 (18)
C13—N2—C6—O1	172.8 (2)	C26—N4—C19—C20	3.5 (2)
N1—N2—C6—C7	−176.46 (19)	O3—C19—C20—C21	−2.8 (4)
C13—N2—C6—C7	−6.1 (3)	N4—C19—C20—C21	178.0 (2)
O1—C6—C7—C8	5.7 (5)	O3—C19—C20—C25	175.2 (2)
N2—C6—C7—C8	−175.5 (2)	N4—C19—C20—C25	−4.0 (2)
O1—C6—C7—C12	−174.4 (3)	C25—C20—C21—C22	−1.1 (4)
N2—C6—C7—C12	4.4 (3)	C19—C20—C21—C22	176.7 (2)
C12—C7—C8—C9	0.2 (4)	C20—C21—C22—C23	−0.3 (4)
C6—C7—C8—C9	−179.9 (2)	C21—C22—C23—C24	1.4 (4)
C7—C8—C9—C10	1.4 (4)	C22—C23—C24—C25	−1.0 (4)
C8—C9—C10—C11	−1.4 (4)	C23—C24—C25—C20	−0.5 (3)
C9—C10—C11—C12	−0.1 (4)	C23—C24—C25—C26	180.0 (2)
C10—C11—C12—C7	1.7 (4)	C21—C20—C25—C24	1.5 (4)
C10—C11—C12—C13	−178.9 (3)	C19—C20—C25—C24	−176.7 (2)
C8—C7—C12—C11	−1.8 (4)	C21—C20—C25—C26	−178.8 (2)
C6—C7—C12—C11	178.3 (2)	C19—C20—C25—C26	3.0 (3)
C8—C7—C12—C13	178.7 (2)	N3—N4—C26—O4	7.5 (4)
C6—C7—C12—C13	−1.2 (3)	C19—N4—C26—O4	177.9 (2)
N1—N2—C13—O2	−3.6 (4)	N3—N4—C26—C25	−172.2 (2)
C6—N2—C13—O2	−172.6 (3)	C19—N4—C26—C25	−1.8 (2)
N1—N2—C13—C12	174.4 (2)	C24—C25—C26—O4	−0.9 (4)
C6—N2—C13—C12	5.4 (3)	C20—C25—C26—O4	179.4 (2)
C11—C12—C13—O2	−4.0 (5)	C24—C25—C26—N4	178.8 (2)
C7—C12—C13—O2	175.5 (3)	C20—C25—C26—N4	−0.9 (2)

Fig. 1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O3

Fig. 2