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4,6-Dimethoxy-2-(methylsulfanyl)-5-phenylpyrimidine

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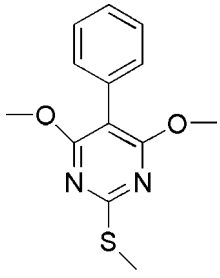
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.176; data-to-parameter ratio = 17.4.

In the asymmetric unit of the title structure, $C_{13}H_{14}N_2O_2S$, there are two independent molecules. All bond lengths and angles show normal values. The dihedral angles between the phenyl and pyrimidine rings in each molecule are 58.66 (9) and 57.88 (8)°, but these rings are rotated in opposite directions with respect to the S—C bond of the methylsulfanyl substituent. In the absence of hydrogen bonds, the crystal structure is stabilized by van der Waals forces and one weak C—H···π(arene) interaction, with H···Cg = 2.91 Å (Cg is the centroid of the pyrimidine ring).

Related literature

Pyrimidine derivatives have been studied because of their biological properties (see Koppel *et al.*, 1961; Zhang & Wang, 1988; Nezu & Miyazaki, 1996).



Experimental

Crystal data

$C_{13}H_{14}N_2O_2S$
M_r = 262.32
Monoclinic, $P2_1/c$
a = 8.4346 (5) Å
b = 35.193 (2) Å
c = 9.4327 (6) Å
β = 109.356 (1)°
V = 2641.7 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 296 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
18638 measured reflections
5743 independent reflections
3710 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.177
S = 1.01
5743 reflections
331 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2421).

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supplementary materials

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4,6-Dimethoxy-2-(methylsulfanyl)-5-phenylpyrimidine

T.-H. Huang, N. Zhao, L.-F. Chen, H.-G. Cheng and F.-H. Luo

Comment

Pyrimidine derivates are important intermediates for some pesticides. Many new pyrimidine derivates have been intensively studied due to their biological properties (Koppel *et al.*, 1961; Zhang *et al.*, 1988; Nezu *et al.*, 1996). We report here the synthesis and crystal structure of the title compound (Fig. 1).

There are two independent molecules in the asymmetric unit of the title structure (Fig. 1). The molecules differ from each other in that the dihedral angles between the phenyl ring and pyrimidine ring in each molecule are 58.66 (9)° and 57.88 (8)° but these are in the opposite sense with respect to the S—C bond of methylthio substituent. In the crystal structure, no hydrogen bonds are found, and the crystal packing is stabilized by van der Waals forces and one very weak C—H···π(arene) interaction with H7A···*Cg* = 2.91 Å, C7···*Cg* = 3.373 (3)Å and C7—H7A···*Cg* = 128° (Fig. 2). *Cg* is the centroid defined by the atoms of the pyrimidine ring.

Experimental

To a solution of 4,6-dichloro-2-(methylthio)-5-phenylpyrimidine (10 mmol) in absolute Methanol (20 ml), a solution of sodium methoxide (20 mmol) in absolute methanol (20 ml) was added dropwise and refluxed for 6 h. After this time the reaction mixture was concentrated to a residual solid. The solid was dissolved in 50 ml of ethyl acetate, washed with water, dried and evaporated under reduced pressure to give a white solid. The solid was recrystallized from CH_2Cl_2. Colourless block-shaped crystals were obtained by evaporation of the solvent over a period of one week.

Refinement

After their location in the difference map, all H-atoms were fixed geometrically at ideal positions and allowed to ride on the parent C atoms with $C_{aromatic}$—H = 0.93Å and C_{methyl}—H = 0.96 Å, U_{iso}(H)= 1.2U_{eq}(C of aromatic) or U_{iso}(H)= 1.5U_{eq}(C of methine).

Figures

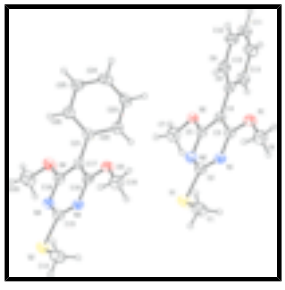


Fig. 1. Molecular structure of (I) showing 30% probability displacement ellipsoids.

Fig. 2. Partial packing plot of (I) with dashed lines indicating C—H···π) interactions.

4,6-Dimethoxy-2-(methylsulfanyl)-5-phenylpyrimidine

Crystal data

$C_{13}H_{14}N_2O_2S$	$Z = 8$
$M_r = 262.32$	$F_{000} = 1104$
Monoclinic, $P2_1/c$	$D_x = 1.319$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.4346$ (5) Å	$\mu = 0.24$ mm^{-1}
$b = 35.193$ (2) Å	$T = 296$ (2) K
$c = 9.4327$ (6) Å	Block, colorless
$\beta = 109.356$ (1)º	0.30 × 0.20 × 0.20 mm
$V = 2641.7$ (3) Å^3	

Data collection

Bruker SMART CCD diffractometer	3710 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.062$
Monochromator: graphite	$\theta_{max} = 27.0$º
$T = 296$(2) K	$\theta_{min} = 1.2$º
φ and ω scans	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -37 \rightarrow 44$
18638 measured reflections	$l = -10 \rightarrow 12$
5743 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.060$	H-atom parameters constrained
$wR(F^2) = 0.177$	$w = 1/[\sigma^2(F_o^2) + (0.0932P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
5743 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
331 parameters	$\Delta\rho_{min} = -0.24$ 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}
C1	0.5206 (4)	0.01414 (8)	0.2874 (4)	0.0781 (10)
H1A	0.4782	0.0030	0.3605	0.117*
H1B	0.5425	−0.0055	0.2257	0.117*
H1C	0.4389	0.0315	0.2255	0.117*
C2	0.6413 (3)	0.07590 (7)	0.4721 (3)	0.0467 (6)
C3	0.4358 (3)	0.10674 (7)	0.5265 (3)	0.0462 (6)
C4	0.5431 (3)	0.13661 (6)	0.5940 (3)	0.0432 (6)
C5	0.7097 (3)	0.13073 (7)	0.6023 (3)	0.0442 (6)
C6	0.1651 (4)	0.07707 (8)	0.4594 (4)	0.0683 (8)
H6A	0.1612	0.0741	0.3571	0.102*
H6B	0.0537	0.0815	0.4618	0.102*
H6C	0.2097	0.0544	0.5147	0.102*
C7	0.9994 (4)	0.15082 (8)	0.6860 (3)	0.0660 (8)
H7A	1.0327	0.1262	0.7293	0.099*
H7B	1.0733	0.1698	0.7463	0.099*
H7C	1.0053	0.1514	0.5861	0.099*
C8	0.4815 (3)	0.17163 (6)	0.6455 (3)	0.0440 (6)
C9	0.3554 (3)	0.19274 (7)	0.5434 (3)	0.0512 (6)
H9	0.3095	0.1844	0.4446	0.061*
C10	0.2978 (4)	0.22587 (7)	0.5873 (3)	0.0600 (7)
H10	0.2150	0.2400	0.5172	0.072*
C11	0.3608 (4)	0.23809 (7)	0.7319 (3)	0.0602 (8)
H11	0.3210	0.2604	0.7606	0.072*
C12	0.4838 (4)	0.21730 (8)	0.8360 (3)	0.0617 (7)
H12	0.5259	0.2254	0.9353	0.074*
C13	0.5447 (3)	0.18427 (7)	0.7929 (3)	0.0529 (7)
H13	0.6286	0.1705	0.8633	0.063*
C14	0.9765 (4)	0.00837 (8)	−0.2144 (3)	0.0736 (9)
H14A	0.9293	−0.0006	−0.1408	0.110*
H14B	1.0017	−0.0129	−0.2669	0.110*
H14C	0.8972	0.0247	−0.2846	0.110*
C15	1.0923 (3)	0.07136 (7)	−0.0362 (3)	0.0453 (6)
C16	0.8881 (3)	0.10212 (6)	0.0210 (3)	0.0402 (5)

C17	0.9962 (3)	0.13147 (6)	0.0897 (2)	0.0384 (5)
C18	1.1608 (3)	0.12611 (7)	0.0919 (3)	0.0432 (6)
C19	0.6142 (3)	0.07471 (8)	−0.0560 (3)	0.0650 (8)
H19A	0.6173	0.0715	−0.1562	0.097*
H19B	0.5021	0.0811	−0.0603	0.097*
H19C	0.6478	0.0515	−0.0011	0.097*
C20	1.4415 (3)	0.14925 (9)	0.1545 (4)	0.0789 (10)
H20A	1.4914	0.1264	0.2057	0.118*
H20B	1.5077	0.1708	0.2024	0.118*
H20C	1.4371	0.1480	0.0516	0.118*
C21	0.9432 (3)	0.16609 (6)	0.1519 (2)	0.0384 (5)
C22	0.8676 (3)	0.16418 (7)	0.2617 (3)	0.0466 (6)
H22	0.8507	0.1407	0.2997	0.056*
C23	0.8170 (3)	0.19721 (7)	0.3150 (3)	0.0535 (7)
H23	0.7682	0.1957	0.3900	0.064*
C24	0.8379 (3)	0.23174 (7)	0.2590 (3)	0.0554 (7)
H24	0.8008	0.2536	0.2937	0.066*
C25	0.9141 (3)	0.23431 (7)	0.1506 (3)	0.0564 (7)
H25	0.9305	0.2579	0.1134	0.068*
C26	0.9659 (3)	0.20179 (7)	0.0979 (3)	0.0506 (6)
H26	1.0172	0.2037	0.0248	0.061*
N1	0.4813 (3)	0.07636 (5)	0.4644 (2)	0.0476 (5)
N2	0.7612 (3)	0.10095 (6)	0.5409 (2)	0.0478 (5)
N3	0.9330 (2)	0.07204 (5)	−0.0438 (2)	0.0434 (5)
N4	1.2120 (3)	0.09663 (6)	0.0305 (2)	0.0473 (5)
O1	0.2716 (2)	0.10897 (5)	0.5267 (2)	0.0556 (5)
O2	0.8297 (2)	0.15852 (4)	0.68017 (19)	0.0481 (4)
O3	0.7269 (2)	0.10457 (4)	0.0178 (2)	0.0515 (5)
O4	1.2743 (2)	0.15312 (5)	0.1602 (2)	0.0578 (5)
S1	0.70988 (10)	0.03907 (2)	0.38070 (9)	0.0662 (3)
S2	1.16403 (10)	0.03415 (2)	−0.12325 (9)	0.0657 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.082 (2)	0.066 (2)	0.089 (2)	−0.0102 (17)	0.0320 (19)	−0.0344 (17)
C2	0.0509 (15)	0.0433 (14)	0.0479 (14)	0.0042 (12)	0.0190 (12)	−0.0002 (11)
C3	0.0505 (15)	0.0394 (14)	0.0518 (14)	0.0011 (12)	0.0211 (12)	0.0007 (11)
C4	0.0492 (15)	0.0383 (13)	0.0452 (13)	0.0035 (11)	0.0197 (12)	0.0004 (10)
C5	0.0517 (15)	0.0397 (14)	0.0446 (13)	0.0019 (12)	0.0205 (12)	0.0020 (10)
C6	0.0492 (17)	0.0609 (19)	0.095 (2)	−0.0102 (14)	0.0240 (17)	−0.0060 (16)
C7	0.066 (2)	0.0651 (19)	0.0609 (18)	−0.0120 (15)	0.0129 (15)	−0.0033 (14)
C8	0.0504 (15)	0.0369 (13)	0.0489 (14)	−0.0032 (11)	0.0222 (12)	0.0008 (10)
C9	0.0633 (17)	0.0485 (15)	0.0421 (14)	0.0081 (13)	0.0179 (13)	−0.0008 (11)
C10	0.0705 (19)	0.0507 (17)	0.0607 (17)	0.0192 (14)	0.0242 (15)	0.0048 (13)
C11	0.071 (2)	0.0450 (16)	0.073 (2)	0.0071 (14)	0.0353 (17)	−0.0080 (14)
C12	0.0702 (19)	0.0600 (18)	0.0557 (17)	−0.0004 (16)	0.0221 (15)	−0.0166 (14)
C13	0.0517 (15)	0.0550 (16)	0.0488 (15)	0.0045 (13)	0.0125 (13)	0.0004 (12)

C14	0.084 (2)	0.063 (2)	0.074 (2)	0.0017 (17)	0.0248 (18)	−0.0201 (15)
C15	0.0503 (15)	0.0411 (14)	0.0475 (14)	0.0045 (12)	0.0203 (12)	0.0009 (11)
C16	0.0379 (13)	0.0365 (13)	0.0462 (13)	0.0027 (10)	0.0141 (11)	0.0041 (10)
C17	0.0391 (13)	0.0379 (13)	0.0399 (12)	0.0017 (10)	0.0152 (11)	−0.0004 (10)
C18	0.0404 (14)	0.0470 (14)	0.0436 (13)	−0.0018 (11)	0.0156 (11)	−0.0013 (11)
C19	0.0462 (16)	0.0584 (18)	0.087 (2)	−0.0138 (14)	0.0181 (15)	−0.0114 (15)
C20	0.0435 (17)	0.085 (2)	0.112 (3)	−0.0153 (16)	0.0311 (18)	−0.0227 (19)
C21	0.0311 (12)	0.0418 (13)	0.0382 (12)	−0.0020 (10)	0.0061 (10)	−0.0048 (10)
C22	0.0455 (15)	0.0495 (15)	0.0462 (14)	−0.0041 (12)	0.0169 (12)	0.0004 (11)
C23	0.0527 (16)	0.0595 (17)	0.0529 (15)	−0.0054 (13)	0.0237 (13)	−0.0145 (13)
C24	0.0505 (16)	0.0483 (16)	0.0625 (17)	0.0052 (13)	0.0120 (14)	−0.0179 (13)
C25	0.0703 (19)	0.0385 (15)	0.0580 (16)	0.0031 (13)	0.0178 (15)	−0.0024 (12)
C26	0.0593 (16)	0.0464 (15)	0.0494 (15)	−0.0027 (13)	0.0225 (13)	0.0008 (11)
N1	0.0507 (13)	0.0362 (11)	0.0597 (13)	0.0018 (10)	0.0235 (11)	−0.0034 (9)
N2	0.0481 (12)	0.0454 (12)	0.0516 (12)	0.0038 (10)	0.0186 (10)	−0.0031 (10)
N3	0.0457 (12)	0.0346 (11)	0.0512 (12)	0.0005 (9)	0.0178 (10)	−0.0027 (9)
N4	0.0427 (12)	0.0467 (12)	0.0561 (13)	0.0002 (10)	0.0211 (10)	−0.0064 (10)
O1	0.0406 (10)	0.0425 (10)	0.0877 (14)	−0.0076 (8)	0.0268 (10)	−0.0151 (9)
O2	0.0437 (10)	0.0442 (10)	0.0645 (11)	0.0033 (8)	0.0289 (9)	0.0021 (8)
O3	0.0379 (9)	0.0402 (10)	0.0764 (12)	−0.0042 (8)	0.0190 (9)	−0.0122 (8)
O4	0.0366 (10)	0.0630 (12)	0.0756 (13)	−0.0105 (9)	0.0211 (9)	−0.0242 (9)
S1	0.0610 (5)	0.0613 (5)	0.0785 (5)	0.0068 (4)	0.0261 (4)	−0.0220 (4)
S2	0.0670 (5)	0.0558 (5)	0.0830 (5)	0.0042 (4)	0.0364 (4)	−0.0186 (4)

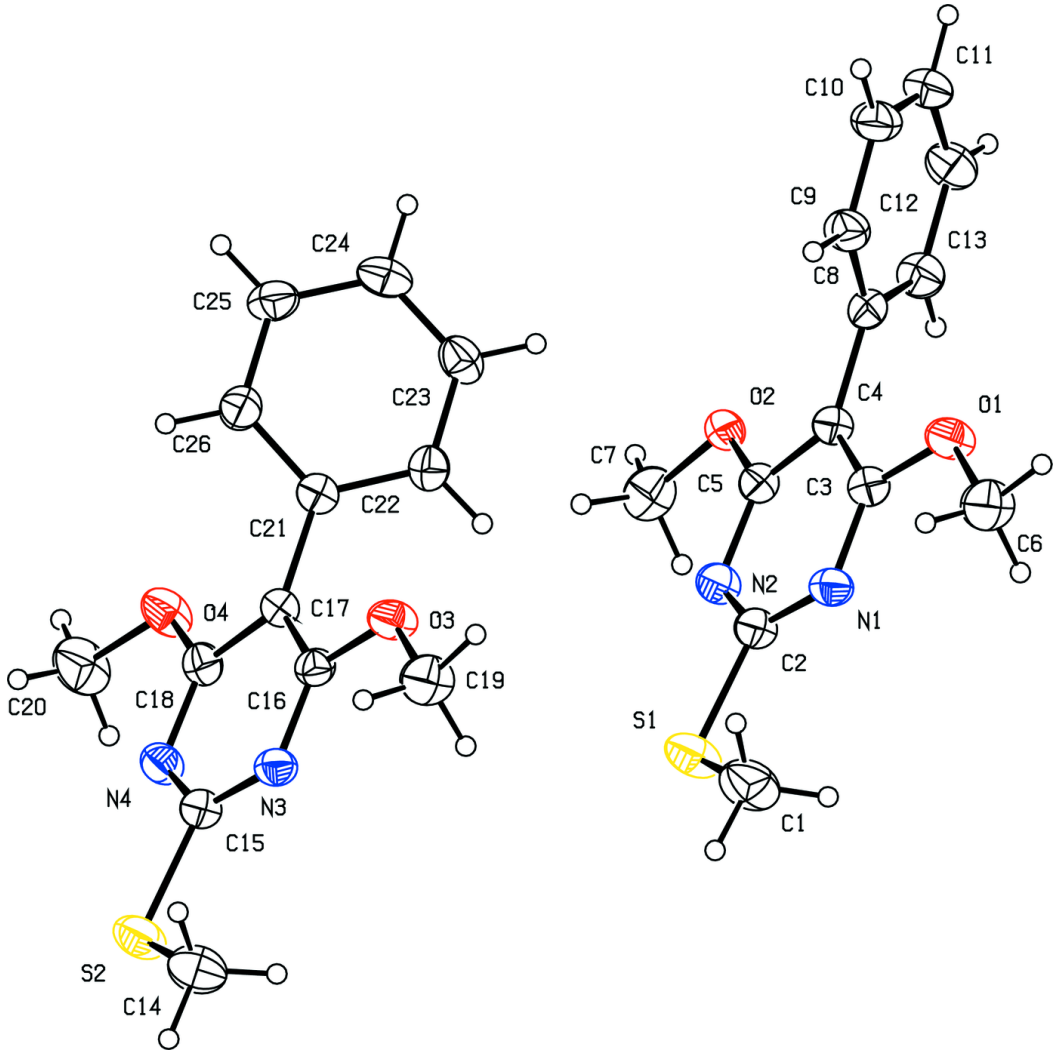
Geometric parameters (Å, °)

C1—S1	1.778 (3)	C14—S2	1.779 (3)
C1—H1A	0.9600	C14—H14A	0.9600
C1—H1B	0.9600	C14—H14B	0.9600
C1—H1C	0.9600	C14—H14C	0.9600
C2—N1	1.328 (3)	C15—N3	1.322 (3)
C2—N2	1.336 (3)	C15—N4	1.336 (3)
C2—S1	1.757 (2)	C15—S2	1.756 (2)
C3—N1	1.335 (3)	C16—N3	1.338 (3)
C3—O1	1.387 (3)	C16—O3	1.353 (3)
C3—C4	1.395 (3)	C16—C17	1.388 (3)
C4—C5	1.397 (3)	C17—C18	1.394 (3)
C4—C8	1.481 (3)	C17—C21	1.484 (3)
C5—N2	1.338 (3)	C18—N4	1.328 (3)
C5—O2	1.425 (3)	C18—O4	1.352 (3)
C6—O1	1.447 (3)	C19—O3	1.433 (3)
C6—H6A	0.9600	C19—H19A	0.9600
C6—H6B	0.9600	C19—H19B	0.9600
C6—H6C	0.9600	C19—H19C	0.9600
C7—O2	1.439 (3)	C20—O4	1.435 (3)
C7—H7A	0.9600	C20—H20A	0.9600
C7—H7B	0.9600	C20—H20B	0.9600
C7—H7C	0.9600	C20—H20C	0.9600
C8—C13	1.387 (3)	C21—C22	1.386 (3)

C8—C9	1.390 (3)	C21—C26	1.392 (3)
C9—C10	1.378 (3)	C22—C23	1.389 (3)
C9—H9	0.9300	C22—H22	0.9300
C10—C11	1.360 (4)	C23—C24	1.360 (3)
C10—H10	0.9300	C23—H23	0.9300
C11—C12	1.379 (4)	C24—C25	1.379 (4)
C11—H11	0.9300	C24—H24	0.9300
C12—C13	1.385 (3)	C25—C26	1.376 (3)
C12—H12	0.9300	C25—H25	0.9300
C13—H13	0.9300	C26—H26	0.9300
S1—C1—H1A	109.5	H14B—C14—H14C	109.5
S1—C1—H1B	109.5	N3—C15—N4	127.6 (2)
H1A—C1—H1B	109.5	N3—C15—S2	119.31 (19)
S1—C1—H1C	109.5	N4—C15—S2	113.13 (17)
H1A—C1—H1C	109.5	N3—C16—O3	118.3 (2)
H1B—C1—H1C	109.5	N3—C16—C17	124.1 (2)
N1—C2—N2	127.6 (2)	O3—C16—C17	117.5 (2)
N1—C2—S1	118.43 (19)	C16—C17—C18	113.7 (2)
N2—C2—S1	113.94 (18)	C16—C17—C21	124.0 (2)
N1—C3—O1	118.6 (2)	C18—C17—C21	122.2 (2)
N1—C3—C4	124.5 (2)	N4—C18—O4	118.4 (2)
O1—C3—C4	117.0 (2)	N4—C18—C17	124.4 (2)
C3—C4—C5	113.7 (2)	O4—C18—C17	117.2 (2)
C3—C4—C8	122.1 (2)	O3—C19—H19A	109.5
C5—C4—C8	124.1 (2)	O3—C19—H19B	109.5
N2—C5—C4	123.9 (2)	H19A—C19—H19B	109.5
N2—C5—O2	118.9 (2)	O3—C19—H19C	109.5
C4—C5—O2	117.2 (2)	H19A—C19—H19C	109.5
O1—C6—H6A	109.5	H19B—C19—H19C	109.5
O1—C6—H6B	109.5	O4—C20—H20A	109.5
H6A—C6—H6B	109.5	O4—C20—H20B	109.5
O1—C6—H6C	109.5	H20A—C20—H20B	109.5
H6A—C6—H6C	109.5	O4—C20—H20C	109.5
H6B—C6—H6C	109.5	H20A—C20—H20C	109.5
O2—C7—H7A	109.5	H20B—C20—H20C	109.5
O2—C7—H7B	109.5	C22—C21—C26	118.0 (2)
H7A—C7—H7B	109.5	C22—C21—C17	121.9 (2)
O2—C7—H7C	109.5	C26—C21—C17	120.0 (2)
H7A—C7—H7C	109.5	C21—C22—C23	120.2 (2)
H7B—C7—H7C	109.5	C21—C22—H22	119.9
C13—C8—C9	118.4 (2)	C23—C22—H22	119.9
C13—C8—C4	122.4 (2)	C24—C23—C22	120.8 (2)
C9—C8—C4	119.2 (2)	C24—C23—H23	119.6
C10—C9—C8	120.6 (2)	C22—C23—H23	119.6
C10—C9—H9	119.7	C23—C24—C25	119.9 (2)
C8—C9—H9	119.7	C23—C24—H24	120.0
C11—C10—C9	120.6 (3)	C25—C24—H24	120.0
C11—C10—H10	119.7	C26—C25—C24	119.7 (2)
C9—C10—H10	119.7	C26—C25—H25	120.2

C10—C11—C12	119.9 (2)	C24—C25—H25	120.2
C10—C11—H11	120.1	C25—C26—C21	121.3 (2)
C12—C11—H11	120.1	C25—C26—H26	119.3
C11—C12—C13	120.1 (3)	C21—C26—H26	119.3
C11—C12—H12	120.0	C2—N1—C3	114.9 (2)
C13—C12—H12	120.0	C2—N2—C5	115.1 (2)
C12—C13—C8	120.4 (2)	C15—N3—C16	115.2 (2)
C12—C13—H13	119.8	C18—N4—C15	114.9 (2)
C8—C13—H13	119.8	C3—O1—C6	115.49 (19)
S2—C14—H14A	109.5	C5—O2—C7	114.72 (18)
S2—C14—H14B	109.5	C16—O3—C19	117.65 (19)
H14A—C14—H14B	109.5	C18—O4—C20	117.71 (19)
S2—C14—H14C	109.5	C2—S1—C1	102.66 (13)
H14A—C14—H14C	109.5	C15—S2—C14	102.54 (13)
N1—C3—C4—C5	−4.9 (4)	C21—C22—C23—C24	1.1 (4)
O1—C3—C4—C5	174.3 (2)	C22—C23—C24—C25	−1.7 (4)
N1—C3—C4—C8	172.8 (2)	C23—C24—C25—C26	1.2 (4)
O1—C3—C4—C8	−8.0 (3)	C24—C25—C26—C21	−0.1 (4)
C3—C4—C5—N2	5.2 (3)	C22—C21—C26—C25	−0.5 (4)
C8—C4—C5—N2	−172.4 (2)	C17—C21—C26—C25	178.3 (2)
C3—C4—C5—O2	−175.19 (19)	N2—C2—N1—C3	3.9 (4)
C8—C4—C5—O2	7.2 (3)	S1—C2—N1—C3	−175.03 (18)
C3—C4—C8—C13	123.0 (3)	O1—C3—N1—C2	−178.4 (2)
C5—C4—C8—C13	−59.5 (3)	C4—C3—N1—C2	0.7 (4)
C3—C4—C8—C9	−56.8 (3)	N1—C2—N2—C5	−3.5 (4)
C5—C4—C8—C9	120.7 (3)	S1—C2—N2—C5	175.44 (17)
C13—C8—C9—C10	1.5 (4)	C4—C5—N2—C2	−1.5 (3)
C4—C8—C9—C10	−178.7 (2)	O2—C5—N2—C2	178.9 (2)
C8—C9—C10—C11	−1.3 (4)	N4—C15—N3—C16	1.4 (4)
C9—C10—C11—C12	0.2 (4)	S2—C15—N3—C16	−177.72 (17)
C10—C11—C12—C13	0.9 (4)	O3—C16—N3—C15	−179.8 (2)
C11—C12—C13—C8	−0.7 (4)	C17—C16—N3—C15	1.3 (3)
C9—C8—C13—C12	−0.4 (4)	O4—C18—N4—C15	−179.4 (2)
C4—C8—C13—C12	179.7 (2)	C17—C18—N4—C15	0.0 (4)
N3—C16—C17—C18	−2.9 (3)	N3—C15—N4—C18	−2.0 (4)
O3—C16—C17—C18	178.2 (2)	S2—C15—N4—C18	177.13 (17)
N3—C16—C17—C21	175.5 (2)	N1—C3—O1—C6	0.8 (3)
O3—C16—C17—C21	−3.5 (3)	C4—C3—O1—C6	−178.4 (2)
C16—C17—C18—N4	2.2 (3)	N2—C5—O2—C7	−0.8 (3)
C21—C17—C18—N4	−176.2 (2)	C4—C5—O2—C7	179.6 (2)
C16—C17—C18—O4	−178.4 (2)	N3—C16—O3—C19	−0.3 (3)
C21—C17—C18—O4	3.2 (3)	C17—C16—O3—C19	178.7 (2)
C16—C17—C21—C22	57.7 (3)	N4—C18—O4—C20	3.5 (3)
C18—C17—C21—C22	−124.1 (3)	C17—C18—O4—C20	−175.9 (2)
C16—C17—C21—C26	−121.0 (3)	N1—C2—S1—C1	4.6 (2)
C18—C17—C21—C26	57.2 (3)	N2—C2—S1—C1	−174.5 (2)
C26—C21—C22—C23	−0.1 (3)	N3—C15—S2—C14	4.3 (2)
C17—C21—C22—C23	−178.8 (2)	N4—C15—S2—C14	−174.90 (19)

Fig. 1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S2
C14

Fig. 2