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(*Z*)-2-[2-(Cyanoimino)-1,3-thiazolidin-1-yl]-1,3-diphenylprop-2-en-1-one

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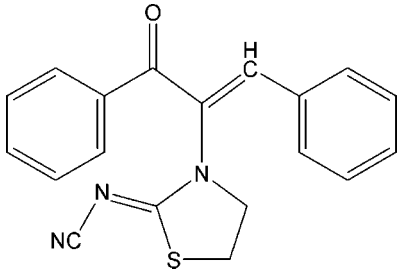
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.044; wR factor = 0.108; data-to-parameter ratio = 14.0.

In the title compound, $C_{19}H_{15}N_3OS$, the 2-(cyanoimino)thiazolidine unit is approximately planar and makes dihedral angles of 63.74 (13) and 68.56 (15)° with the plane of the benzoyl C atoms and the benzylidene phenyl ring, respectively. In the crystal structure, a weak intermolecular C—H···O interaction is observed.

Related literature

For related literature, see: Ezer *et al.* (1984); Honda *et al.* (2006); Klein (2001); Liu *et al.* (2006); Müller *et al.* (2002); Ogawa (2000); Oliver *et al.* (2005); Schmuck *et al.* (2003); Shiokawa *et al.* (1990); Yoneda *et al.* (2001).



Experimental

Crystal data

$C_{19}H_{15}N_3OS$
M_r = 333.40
Monoclinic, $P2_1$
a = 9.927 (4) Å
b = 8.389 (4) Å
c = 10.883 (5) Å
β = 112.660 (8)°
V = 836.3 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.12 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.966, T_{max} = 0.976
4284 measured reflections
2864 independent reflections
2018 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 1.03
2864 reflections
205 parameters
19 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1288 Friedel pairs
Flack parameter: 0.04 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16B···O1^{i}	0.97	2.39	3.300 (5)	156

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+1$.

Data collection: *SMART* (Bruker, 1998); 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, 1999); 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: IS2212).

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supplementary materials

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(*Z*)-2-[2-(Cyanoimino)-1,3-thiazolidin-1-yl]-1,3-diphenylprop-2-en-1-one

H. Dai, X. Zhang, X. Qin, Z.-F. Qin and J.-X. Fang

Comment

Thiazolidine derivatives are reported to possess various biological activities and physiological activities, such as antihypertensive, vasodilator, antiulcer, insecticidal and herbicidal activities (Shiokawa *et al.*, 1990; Ezer *et al.*, 1984; Ogawa, 2000; Müller *et al.*, 2002; Schmuck *et al.*, 2003). They are becoming more and more important in the development of medicines and agriculture. (Honda *et al.*, 2006; Yoneda *et al.*, 2001; Klein, 2001; Oliver *et al.*, 2005). In order to investigate novel biological compounds containing the 2-cyanoiminothiazolidine group, we designed and synthesized the title compound, (I).

Figure 1 shows the molecular structure of (I), which contains three planar rings: the phenyl ring (p1: C1—C6), the 1,3-thiazolidine ring (p2: S1/C18/N1/C16/C17), and the other phenyl ring (p3: C10—C15). The dihedral angles between p1 and p2, and between p3 and p2 are 64.9 (2) and 67.73 (18)°, respectively. The molecules are linked by intermolecular C—H···O hydrogen bonds (Fig. 2).

Experimental

To a stirred solution of 3-[(2-oxo-2-phenylethyl)thiazolidin-2-ylideneamino] formonitrile (2.45 g, 10 mmol; Liu *et al.*, 2006), benzaldehyde (1.27 g, 12 mmol) and anhydrous toluene (30 ml) were added a few drops of piperidine at room temperature under nitrogen. The mixture was heated to reflux for 5 h. The solvent was evaporated under reduced pressure and the residue was then purified by column chromatography on silica gel (200–300 mesh), with petroleum ether/ethyl acetate (4:1 *v*/*v*) as eluent. The resulting yellow solid was recrystallized from petroleum ether/ethyl acetate (2:3 *v*/*v*) to give yellow crystals (yield 76%).

Refinement

The displacement parameters of atoms C12, C13 and C14 were restrained to behave approximately isotropic. The phenyl ring of C10—C15 was constrained as a hexagon with the C—C bonds of 1.39 Å. H atoms were placed in calculated positions (C—H = 0.93 or 0.97 Å) and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

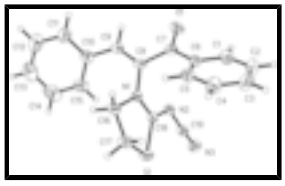

Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

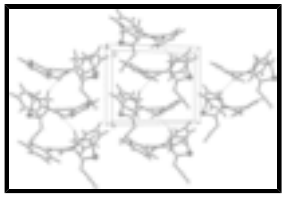

Fig. 2. Packing diagram of the title compound. Dashed lines indicate C—H···O hydrogen-bond interactions.

(*Z*)-2-[2-(Cyanoimino)-1,3-thiazolidin-1-yl]-1,3-diphenylprop-2-en-1-one

Crystal data

$C_{19}H_{15}N_3OS$	F_{000} = 348
M_r = 333.40	D_x = 1.324 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 1300 reflections
a = 9.927 (4) Å	θ = 3.2–22.7º
b = 8.389 (4) Å	μ = 0.20 mm^{-1}
c = 10.883 (5) Å	T = 294 (2) K
β = 112.660 (8)º	Monoclinic, yellow
V = 836.3 (7) Å^3	0.20 × 0.18 × 0.12 mm
Z = 2	

Data collection

Bruker SMART 1000 diffractometer	2864 independent reflections
Radiation source: fine-focus sealed tube	2018 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −9→11
T_{min} = 0.966, T_{max} = 0.976	k = −9→9
4284 measured reflections	l = −11→12

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.0872P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.108	$(\Delta/\sigma)_{max}$ = 0.003
S = 1.03	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
2864 reflections	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
205 parameters	Extinction correction: none
19 restraints	Absolute structure: Flack (1983), 1288 Friedel pairs

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Flack parameter: 0.04 (11)

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	0.93482 (9)	0.39396 (12)	0.89044 (9)	0.0501 (3)
O1	0.3637 (2)	0.3867 (4)	0.4751 (2)	0.0626 (7)
N1	0.7396 (3)	0.3105 (3)	0.6658 (3)	0.0377 (7)
N2	0.7006 (3)	0.5630 (4)	0.7268 (3)	0.0431 (8)
N3	0.7699 (3)	0.7903 (4)	0.8818 (3)	0.0588 (9)
C1	0.3495 (4)	0.3343 (5)	0.7246 (4)	0.0657 (12)
H1	0.2937	0.4191	0.6762	0.079*
C2	0.3285 (5)	0.2780 (7)	0.8354 (5)	0.0810 (15)
H2	0.2601	0.3266	0.8622	0.097*
C3	0.4074 (6)	0.1520 (7)	0.9055 (5)	0.0781 (14)
H3	0.3928	0.1151	0.9801	0.094*
C4	0.5074 (5)	0.0796 (6)	0.8668 (5)	0.0676 (12)
H4	0.5593	−0.0083	0.9134	0.081*
C5	0.5313 (4)	0.1379 (4)	0.7574 (4)	0.0507 (10)
H5	0.6016	0.0900	0.7326	0.061*
C6	0.4531 (4)	0.2649 (4)	0.6854 (4)	0.0428 (9)
C7	0.4669 (4)	0.3283 (4)	0.5640 (4)	0.0438 (9)
C8	0.6097 (3)	0.3175 (4)	0.5481 (3)	0.0374 (8)
C9	0.6117 (4)	0.3133 (5)	0.4264 (3)	0.0450 (9)
H9	0.5201	0.3063	0.3578	0.054*
C10	0.7333 (2)	0.3179 (3)	0.3828 (3)	0.0506 (9)
C11	0.7150 (3)	0.2416 (4)	0.2640 (3)	0.0704 (13)
H11	0.6264	0.1932	0.2141	0.085*
C12	0.8290 (4)	0.2376 (4)	0.2199 (3)	0.0958 (17)
H12	0.8167	0.1865	0.1404	0.115*
C13	0.9614 (3)	0.3099 (5)	0.2945 (4)	0.1010 (17)
H13	1.0377	0.3073	0.2649	0.121*
C14	0.9797 (2)	0.3863 (5)	0.4132 (3)	0.0951 (16)
H14	1.0683	0.4347	0.4631	0.114*
C15	0.8657 (3)	0.3903 (4)	0.4574 (2)	0.0708 (12)

H15	0.8780	0.4414	0.5368	0.085*
C16	0.8452 (4)	0.1804 (4)	0.6972 (4)	0.0471 (9)
H16A	0.9097	0.1940	0.6499	0.057*
H16B	0.7955	0.0788	0.6718	0.057*
C17	0.9300 (4)	0.1865 (5)	0.8442 (4)	0.0575 (11)
H17A	1.0281	0.1461	0.8664	0.069*
H17B	0.8826	0.1230	0.8905	0.069*
C18	0.7760 (4)	0.4323 (4)	0.7513 (3)	0.0372 (9)
C19	0.7429 (4)	0.6805 (4)	0.8146 (4)	0.0427 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0462 (5)	0.0512 (6)	0.0383 (5)	0.0047 (5)	0.0000 (4)	−0.0010 (5)
O1	0.0382 (13)	0.0832 (19)	0.0553 (15)	0.0111 (16)	0.0056 (12)	0.0101 (18)
N1	0.0321 (16)	0.0376 (16)	0.0376 (17)	0.0036 (14)	0.0070 (13)	−0.0046 (15)
N2	0.0376 (17)	0.0407 (19)	0.0430 (19)	0.0016 (15)	0.0067 (14)	−0.0083 (14)
N3	0.058 (2)	0.056 (2)	0.054 (2)	0.0010 (18)	0.0134 (16)	−0.0140 (19)
C1	0.058 (3)	0.075 (3)	0.064 (3)	0.012 (2)	0.023 (2)	−0.006 (2)
C2	0.075 (3)	0.110 (4)	0.071 (3)	0.004 (3)	0.044 (3)	−0.018 (3)
C3	0.092 (4)	0.096 (4)	0.057 (3)	−0.005 (3)	0.042 (3)	−0.004 (3)
C4	0.081 (3)	0.063 (3)	0.066 (3)	−0.002 (2)	0.036 (3)	0.004 (2)
C5	0.052 (2)	0.050 (2)	0.054 (3)	−0.0039 (19)	0.024 (2)	−0.004 (2)
C6	0.035 (2)	0.045 (2)	0.046 (2)	−0.0003 (16)	0.0124 (17)	−0.0078 (18)
C7	0.040 (2)	0.042 (2)	0.043 (2)	−0.0030 (17)	0.0091 (17)	−0.0049 (19)
C8	0.0347 (19)	0.0334 (19)	0.035 (2)	−0.0047 (16)	0.0037 (15)	−0.0018 (17)
C9	0.040 (2)	0.047 (2)	0.038 (2)	−0.0022 (17)	0.0038 (16)	0.0017 (18)
C10	0.047 (2)	0.053 (2)	0.047 (2)	0.002 (2)	0.0137 (18)	0.013 (2)
C11	0.076 (3)	0.073 (3)	0.072 (3)	−0.007 (2)	0.039 (3)	−0.011 (3)
C12	0.116 (4)	0.094 (3)	0.101 (3)	0.004 (3)	0.068 (3)	−0.011 (3)
C13	0.093 (3)	0.105 (3)	0.124 (4)	0.007 (3)	0.064 (3)	0.018 (3)
C14	0.070 (3)	0.113 (3)	0.100 (3)	−0.018 (3)	0.030 (2)	0.032 (3)
C15	0.057 (2)	0.097 (3)	0.056 (2)	−0.027 (3)	0.019 (2)	0.006 (3)
C16	0.043 (2)	0.040 (2)	0.051 (2)	0.0080 (17)	0.0091 (18)	−0.0014 (19)
C17	0.052 (3)	0.050 (2)	0.055 (2)	0.009 (2)	0.003 (2)	0.003 (2)
C18	0.0340 (19)	0.042 (2)	0.0357 (19)	0.0011 (15)	0.0129 (15)	0.0002 (16)
C19	0.037 (2)	0.043 (2)	0.043 (2)	0.0045 (17)	0.0097 (17)	0.003 (2)

Geometric parameters (Å, °)

S1—C18	1.744 (3)	C7—C8	1.495 (5)
S1—C17	1.807 (4)	C8—C9	1.333 (5)
O1—C7	1.209 (4)	C9—C10	1.458 (4)
N1—C18	1.335 (4)	C9—H9	0.9300
N1—C8	1.426 (4)	C10—C11	1.3900
N1—C16	1.460 (4)	C10—C15	1.3900
N2—C18	1.296 (4)	C11—C12	1.3900
N2—C19	1.323 (5)	C11—H11	0.9300
N3—C19	1.142 (4)	C12—C13	1.3900

C1—C2	1.384 (6)	C12—H12	0.9300
C1—C6	1.384 (5)	C13—C14	1.3900
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.361 (7)	C14—C15	1.3900
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.361 (6)	C15—H15	0.9300
C3—H3	0.9300	C16—C17	1.495 (5)
C4—C5	1.390 (5)	C16—H16A	0.9700
C4—H4	0.9300	C16—H16B	0.9700
C5—C6	1.373 (5)	C17—H17A	0.9700
C5—H5	0.9300	C17—H17B	0.9700
C6—C7	1.479 (5)		
C18—S1—C17	91.03 (18)	C11—C10—C9	117.5 (2)
C18—N1—C8	120.2 (3)	C15—C10—C9	122.4 (2)
C18—N1—C16	115.6 (3)	C10—C11—C12	120.0
C8—N1—C16	124.1 (3)	C10—C11—H11	120.0
C18—N2—C19	118.9 (3)	C12—C11—H11	120.0
C2—C1—C6	120.3 (4)	C13—C12—C11	120.0
C2—C1—H1	119.9	C13—C12—H12	120.0
C6—C1—H1	119.9	C11—C12—H12	120.0
C3—C2—C1	120.4 (5)	C12—C13—C14	120.0
C3—C2—H2	119.8	C12—C13—H13	120.0
C1—C2—H2	119.8	C14—C13—H13	120.0
C2—C3—C4	120.3 (5)	C15—C14—C13	120.0
C2—C3—H3	119.9	C15—C14—H14	120.0
C4—C3—H3	119.9	C13—C14—H14	120.0
C3—C4—C5	119.6 (5)	C14—C15—C10	120.0
C3—C4—H4	120.2	C14—C15—H15	120.0
C5—C4—H4	120.2	C10—C15—H15	120.0
C6—C5—C4	121.1 (4)	N1—C16—C17	106.4 (3)
C6—C5—H5	119.5	N1—C16—H16A	110.4
C4—C5—H5	119.5	C17—C16—H16A	110.4
C5—C6—C1	118.3 (4)	N1—C16—H16B	110.4
C5—C6—C7	124.2 (3)	C17—C16—H16B	110.4
C1—C6—C7	117.4 (4)	H16A—C16—H16B	108.6
O1—C7—C6	121.3 (3)	C16—C17—S1	105.9 (3)
O1—C7—C8	118.7 (3)	C16—C17—H17A	110.6
C6—C7—C8	120.0 (3)	S1—C17—H17A	110.6
C9—C8—N1	122.5 (3)	C16—C17—H17B	110.6
C9—C8—C7	119.7 (3)	S1—C17—H17B	110.6
N1—C8—C7	117.9 (3)	H17A—C17—H17B	108.7
C8—C9—C10	130.9 (3)	N2—C18—N1	121.6 (3)
C8—C9—H9	114.6	N2—C18—S1	126.3 (3)
C10—C9—H9	114.6	N1—C18—S1	112.1 (2)
C11—C10—C15	120.0	N3—C19—N2	173.7 (4)
C6—C1—C2—C3	−1.3 (7)	C8—C9—C10—C11	151.0 (4)
C1—C2—C3—C4	−0.2 (8)	C8—C9—C10—C15	−26.8 (5)
C2—C3—C4—C5	1.7 (8)	C15—C10—C11—C12	0.0

C3—C4—C5—C6	−1.7 (7)	C9—C10—C11—C12	−177.8 (3)
C4—C5—C6—C1	0.2 (6)	C10—C11—C12—C13	0.0
C4—C5—C6—C7	−176.7 (4)	C11—C12—C13—C14	0.0
C2—C1—C6—C5	1.3 (6)	C12—C13—C14—C15	0.0
C2—C1—C6—C7	178.4 (4)	C13—C14—C15—C10	0.0
C5—C6—C7—O1	147.8 (4)	C11—C10—C15—C14	0.0
C1—C6—C7—O1	−29.1 (5)	C9—C10—C15—C14	177.7 (3)
C5—C6—C7—C8	−30.7 (5)	C18—N1—C16—C17	25.0 (4)
C1—C6—C7—C8	152.4 (3)	C8—N1—C16—C17	−159.2 (3)
C18—N1—C8—C9	117.7 (4)	N1—C16—C17—S1	−30.8 (4)
C16—N1—C8—C9	−57.9 (5)	C18—S1—C17—C16	24.4 (3)
C18—N1—C8—C7	−62.8 (4)	C19—N2—C18—N1	−179.2 (3)
C16—N1—C8—C7	121.6 (4)	C19—N2—C18—S1	−1.4 (5)
O1—C7—C8—C9	−25.1 (5)	C8—N1—C18—N2	−4.2 (5)
C6—C7—C8—C9	153.4 (3)	C16—N1—C18—N2	171.8 (3)
O1—C7—C8—N1	155.4 (4)	C8—N1—C18—S1	177.7 (2)
C6—C7—C8—N1	−26.0 (4)	C16—N1—C18—S1	−6.4 (4)
N1—C8—C9—C10	−7.0 (6)	C17—S1—C18—N2	170.8 (3)
C7—C8—C9—C10	173.5 (4)	C17—S1—C18—N1	−11.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16B···O1^{i}	0.97	2.39	3.300 (5)	156

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

Fig. 1

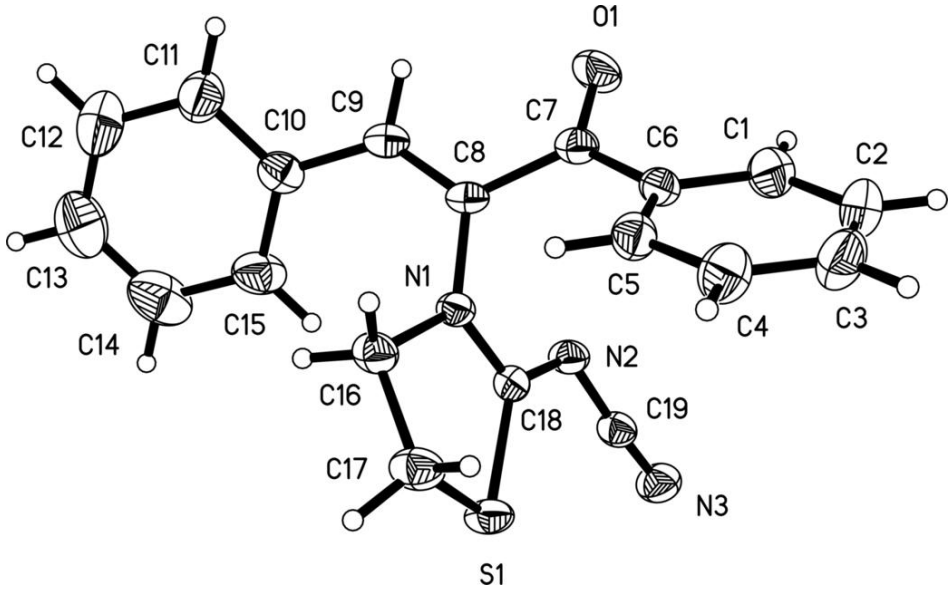
O1
C11
C9
C7
C12
C10
C8
C6
C1
C2
C13
N1
C5
C4
C3
C14
C15
N2
C16
C18
C19
C17
N3
S1

Fig. 2