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5-*tert*-Butyl-2-(*N*,*N*-dimethylaminocarbonylthio)isophthalaldehyde

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The *N*,*N*-dimethylaminocarbonylthio moiety in the title compound, $C_{15}H_{19}NO_3S$, adopts a staggered conformation with respect to the *tert*-butyl substituent in the crystal structure at 180 K.

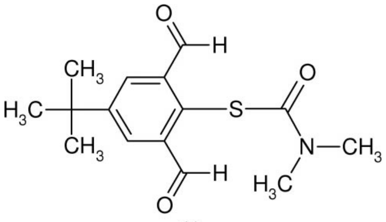
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.112
Data-to-parameter ratio = 25.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The crystal structure of the title compound, (I), is the first example of a *tert*-butyl-substituted isophthalaldehyde and one of very few structures to date that contain the *N*,*N*-dimethylaminocarbonylthio moiety bound to a benzene ring (Bennett *et al.*, 1999; Higgs & Carrano, 2002; Gibbs *et al.*, 1995). The approximately planar *N*,*N*-dimethylaminocarbonylthio group adopts a dihedral angle of 69.0 (1)° to the plane of the benzene ring so that it forms a 'staggered' orientation with respect to the *tert*-butyl group (Fig. 2). The benzene rings of molecules related by translation along [100] are close to coplanar and form pairs of C—H···O contacts between the aldehyde groups (Fig. 3).



(I)

Experimental

The title compound was prepared according to the method of Brooker *et al.* (2000).

Crystal data

$C_{15}H_{19}NO_3S$
M_r = 293.37
Monoclinic, $P2_1/c$
a = 8.5830 (2) Å
b = 18.5242 (4) Å
c = 9.3889 (2) Å
β = 93.359 (1)°
V = 1490.21 (6) Å^3
Z = 4
D_x = 1.308 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7497 reflections
θ = 2.4–29.8°
μ = 0.22 mm^{-1}
T = 180 (2) K
Block, colourless
0.40 × 0.30 × 0.10 mm

Data collection

Bruker–Nonius X8APEX-II CCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
46 511 measured reflections
4716 independent reflections
3651 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 31.0°
$h = -12 \rightarrow 12$
$k = -26 \rightarrow 26$
$l = -13 \rightarrow 13$

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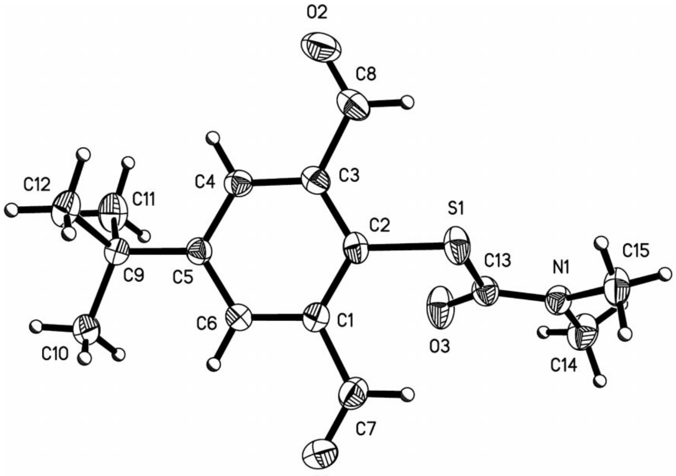

Figure 1
The molecular structure, showing displacement ellipsoids at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

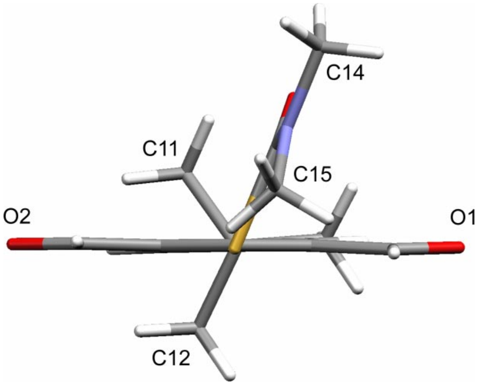

Figure 2
Projection along the C2···C5 vector, showing the staggered arrangement of the *N*,*N*-dimethylaminocarbonylthio group with respect to the *tert*-butyl substituent.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.112$
$S = 1.07$
4716 reflections
186 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.1853P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.40$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

H atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.95 Å and $U_{\rm iso}$(H) = 1.2 $U_{\rm eq}$(C) for Csp^2 atoms, and C—H = 0.98 Å and $U_{\rm iso}$(H) = 1.5 $U_{\rm eq}$(C) for Csp^3. The methyl groups were allowed to rotate about their local threefold axes.

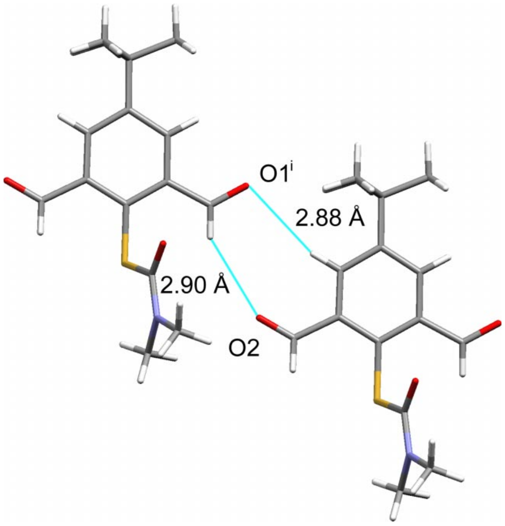

Figure 3
Pairs of C—H···O contacts formed between aldehyde groups. [Symmetry code: (i) 1 + *x*, *y*, *z*.]

Data collection: *APEX*2 (Bruker–Nonius, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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