Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diphenylmethyl 3-azido-1,1-dioxocephalosporanate benzene solvate

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Received 29 August 2006
Accepted 8 September 2006

Key indicators

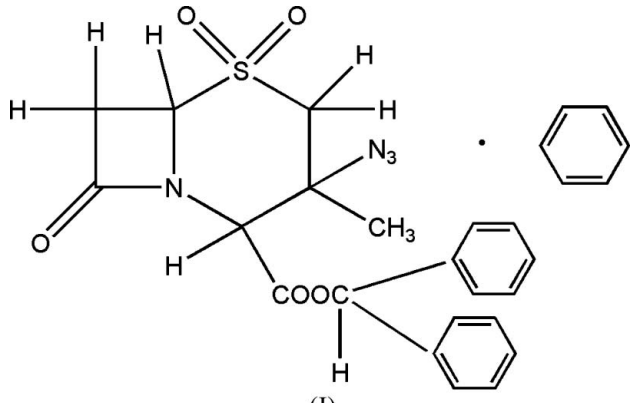
Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.083
Data-to-parameter ratio = 19.2

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

The title compound, $C_{21}H_{20}N_4O_5S\cdot C_6H_6$, is a by-product of the synthesis of tazobactam. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds.

Comment

Tazobactam is a widely used lactamase inhibitor (Micetich *et al.*, 1987). The structure of the title compound, (I), a by-product of the synthesis of tazobactam, is reported here (Fig. 1).



(I)

All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared according to the procedure of Micetich *et al.* (1987) using 6-aminopenicillanic acid as the starting material. Colorless single crystals of (I) were grown by slow evaporation of a benzene solution.

Crystal data

$C_{21}H_{20}N_4O_5S\cdot C_6H_6$
M_r = 518.58
Monoclinic, $P2_1$
a = 8.9971 (17) Å
b = 10.3052 (19) Å
c = 13.954 (3) Å
β = 95.374 (3)°
V = 1288.1 (4) Å^3
Z = 2
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 113 (2) K
Block, colorless
0.32 × 0.20 × 0.14 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.947, T_{max} = 0.971
17106 measured reflections
6459 independent reflections
4755 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 28.7°

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.083$
$S = 0.96$
6459 reflections
337 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.067 (2)
Absolute structure: Flack (1983), 2958 Friedel pairs
Flack parameter: 0.02 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4B···O1^{i}	0.99	2.36	3.266 (2)	152
C8—H8A···O1^{i}	0.98	2.40	3.242 (2)	143
C13—H13···O4^{ii}	0.95	2.48	3.263 (2)	140

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

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.96–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku/MSC, 2005).

Financial support by the Science Project of the Hebei Education Department (grant No. 2005349) is gratefully acknowledged.

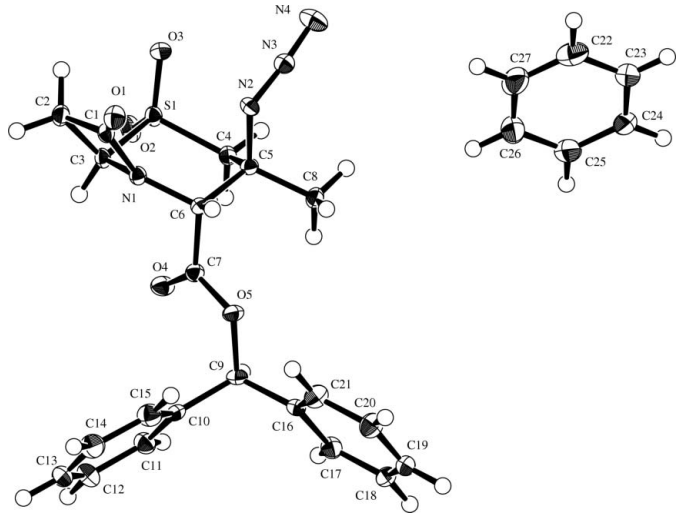

Figure 1
The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

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