fractional coordinates and equivalent isotropic thermal parameters, Table 2 bond distances and selected angles. The molecular structure is shown in Fig. 1.

Related literature. Plešek, Jelínek & Štíbr (1984).

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Structures of Carbocyclic Analogues of Penicillin. 2. *N*-(3,4-Dihydroxy-7-oxobicyclo[3.2.0]hept-6-yl)succinimide

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Abstract. $C_{11}H_{13}NO_5$, $M_r = 239{\cdot}23$, triclinic, $P\bar{1}$, $a = 5{\cdot}470\ (2)$, $b = 6{\cdot}066\ (1)$, $c = 8{\cdot}953\ (2)$ Å, $\alpha = 98{\cdot}55\ (2)$, $\beta = 97{\cdot}31\ (2)$, $\gamma = 113{\cdot}96\ (3)°$, $V = 262{\cdot}6$ Å^3, $Z = 1$, $D_x = 1{\cdot}51$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}92$ mm^{-1}, $F(000) = 126$, $T = 293$ K, $R = 0{\cdot}046$ for 978 unique observed reflections. The determination confirms the chemical structure. The four-membered ring is twisted by 13·4 (4)° and the least-squares best plane through it makes an angle of 108·3 (13)° with the pentane ring. Bond lengths and angles are normal.

Experimental. Material prepared by M. I. Page and G. Cox and crystallized from ethanol. Tabular crystal 0·20 × 0·15 × 0·40 mm. Enraf–Nonius CAD-4*F* diffractometer. No correction for absorption. $2\theta_{max} = 140°$, $+/-h,k,l$; 1917 reflections measured and 41 classed as unobserved ($I < 0$). Check reflection $10\bar{3}$: average count = 9897, calculated σ (of the distribution) = 206 (2·1%). Cell dimensions from θ measurements of 24 reflections ($16 < \theta < 50°$). Data merged using *SHELX*76 (Sheldrick, 1976) giving 991 unique reflections, index range h +/−6, k +/−7, l 0/10; merging $R_{int} = 0{\cdot}026$. *SHELX*76 used to solve structure, by direct methods. Least-squares refinement; 13 reflections, thought to show the effects of extinction, were omitted from the refinement and an anisotropic scale factor (Shakked & Rabinovich, 1977) was used; positional parameters of all atoms and anisotropic thermal vibration parameters for non-H atoms refined; U_{iso} for H fixed at value of U_{eq} of bonded atom; $\sum w(\Delta F)^2$ minimized with $w = 1/\sigma^2(F)$. H atoms from difference Fourier syntheses. In final cycle max. $\Delta/\sigma = 0{\cdot}051$, average = 0·007. $\Delta\rho$ in final difference Fourier map within +0·15 and −0·20 e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). $R = 0{\cdot}046$, $wR = 0{\cdot}058$ for 978 observed reflections [$F_o > 3\sigma(F_o)$].

Atom parameters are given in Table 1,* with bond distances in Table 2. Fig. 1 drawn with *PLUTO*78 (Motherwell & Clegg, 1978) shows the molecule numbering scheme and is a projection along **a**.

* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters, bond angles, torsion angles and best planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43471 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Atom coordinates and e.s.d.'s* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$)

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
C(1)	5633 (10)	4850 (10)	5103 (5)	455
C(2)	7183 (11)	5070 (10)	3784 (6)	488
C(3)	8754 (10)	7870 (9)	3987 (5)	446
C(4)	6813 (10)	8918 (9)	4485 (5)	443
C(5)	5250 (10)	7261 (9)	5494 (5)	458
C(6)	6520 (10)	7572 (9)	7217 (5)	424
C(7)	7472 (11)	5607 (9)	6693 (6)	489
C(8)	11015 (11)	11349 (10)	8290 (6)	461
C(9)	12252 (11)	13297 (10)	9744 (6)	516
C(10)	9979 (12)	12960 (10)	10599 (6)	543
C(11)	7632 (10)	10605 (9)	9687 (6)	472
N(1)	8317	9851	8321	431
O(1)	4815 (9)	8627 (8)	3165 (5)	546
O(2)	9611 (8)	8629 (9)	2630 (5)	582
O(3)	9190 (10)	5060 (9)	7248 (5)	656
O(4)	12120 (9)	11019 (9)	7238 (5)	582
O(5)	5437 (9)	9510 (8)	10037 (5)	569

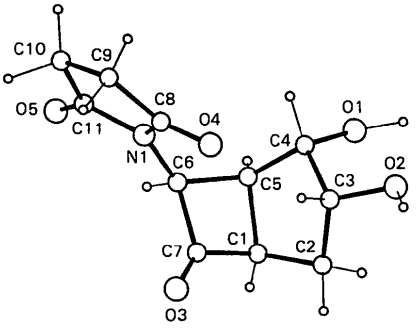

Fig. 1. Diagram of the molecule showing the numbering scheme.

Table 2. *Bond lengths* (Å) *with e.s.d.'s*

C(1)–C(2)	1·530 (6)	C(7)–O(3)	1·193 (5)
C(2)–C(3)	1·529 (6)	C(6)–N(1)	1·448 (5)
C(3)–C(4)	1·521 (5)	N(1)–C(8)	1·391 (5)
C(3)–O(2)	1·430 (5)	N(1)–C(11)	1·390 (5)
C(4)–C(5)	1·525 (5)	C(8)–C(9)	1·489 (5)
C(4)–O(1)	1·440 (4)	C(8)–O(4)	1·216 (5)
C(5)–C(6)	1·560 (5)	C(9)–C(10)	1·502 (7)
C(5)–C(1)	1·555 (6)	C(10)–C(11)	1·501 (6)
C(1)–C(7)	1·522 (5)	C(11)–O(5)	1·221 (5)
C(6)–C(7)	1·520 (6)		

Related literature. This structure is one of a series of β-lactam analogues. Previous structures of the series are listed in Sheldrick, Akrigg, Page & Agathocleous (1985).

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Structures of Carbocyclic Analogues of Penicillin. 3. *N*-(Bicyclo[3.2.0]hept-2-ene-6-spiro-2′-dioxolane-7-yl)phthalimide

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Abstract. $C_{17}H_{15}NO_4$, $M_r = 297{\cdot}31$, triclinic, $P\bar{1}$, $a = 7{\cdot}562$ (2), $b = 8{\cdot}663$ (2), $c = 10{\cdot}979$ (2) Å, $\alpha = 102{\cdot}14$ (1), $\beta = 96{\cdot}86$ (3), $\gamma = 92{\cdot}51$ (3)°, $V = 696{\cdot}35$ Å^3, $Z = 2$, $D_x = 1{\cdot}418$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}74$ mm^{-1}, $F(000) = 312$, $T = 293$ K, $R = 0{\cdot}056$ for 2464 unique observed reflections. The determination confirms the chemical structure. The four-membered ring is twisted by 15·7 (1)° and the

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