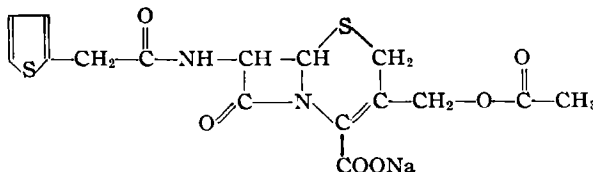


Crystallography of Cephalothin Sodium

By HARRY A. ROSE

CEPHALOTHIN SODIUM is an antibiotic which has shown activity against penicillin resistant organisms. A brief description of the chemistry and microbiological response of the compound has been given elsewhere (1, 2). Data are presented here which permit the identification of this compound by crystallographic methods.

The chemical name of the compound is the sodium salt of 7 (thiophene-2-acetamido) cephalosporanic acid and has the structure



EXPERIMENTAL

This compound can be recrystallized by adding an alcohol to an aqueous solution which results in blades elongated parallel to the *c* axis. The crystals show the prism 110 and the brachypinacoid 010.

The X-ray powder diffraction data were obtained using copper radiation and nickel filter with a camera 114.6 mm. in diameter. A wavelength value of 1.5418 Å. was used in the calculations. The indexing of the powder pattern was done on the basis of single crystal rotation patterns around both the *a* and *c* axes.

TABLE I.—X-RAY DIFFRACTION DATA

Unit cell dimensions: $a_0 = 11.00$ Å., $b_0 = 34.20$ Å., $c_0 = 5.05$ Å.
Formula weights per cell: 4
Formula weight: 418.4
Density: 1.477 Gm./ml. (floatation), 1.463 Gm./ml. (X-ray)
Axial ratio: 0.3216:1:0.1477
Space group: $D_2^2 - P2_12_12_1$

REFERENCES

(1) Chauvette, R. R., *et al.*, *J. Am. Chem. Soc.*, **84**, 3401 (1962).

(2) Boniece, W. S., *et al.*, *J. Bacteriol.*, **84**, 1292(1962).

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TABLE II.—OPTICAL CRYSTALLOGRAPHIC DATA

Refractive indices: $\alpha = 1.568$, $\beta = 1.592$, $\gamma = 1.684$
 Optic axial angle: $\oplus 2V = 56^\circ 34'$ (calcd. from refractive indices)
 Orientation: OAP = 010, $\gamma = a$

TABLE III.—X-RAY POWDER DIFFRACTION DATA

<i>d</i>	<i>I</i> / <i>I</i> ₁	<i>hkl</i>	<i>d</i> (Calcd.)
16.52	0.27	020	17.10
10.53	0.50	110	10.47
9.21	0.50	120	9.25
6.71	0.20	140	6.75
5.71	0.07	060	5.70
5.44	0.07	210	5.43
5.20	0.27	220	5.24
5.05	0.27	160	5.06
4.82	0.07	021	4.84
4.49	1.00b	111, 170, 121	4.55, 4.47, 4.43
4.25	0.67	080, 131	4.28, 4.26
4.05	1.00	051, 141	4.06, 4.04
3.78	0.03	061	3.78
3.67	0.07	211	3.70
3.59	0.03	190, 320	3.59, 3.59
3.49	0.50	071, 330	3.51, 3.49
3.36	0.13	340	3.37
3.24	0.20	081	3.26
3.12	0.20	181	3.13
3.01	0.13	111, 0	2.99
2.91	0.20	210, 0	2.90
2.86	0.03	012, 0	2.85
2.78	0.03	341	2.80
2.72	0.13	420	2.72
2.65	0.07	011, 1	2.65
2.61	0.07	440	2.62
2.53	0.13	002	2.53
2.43	0.03
2.39	0.03
2.36	0.03
2.29	0.07
2.24	0.03