In summary, the results of this analysis suggest the possible mode of action of sulfinpyrazone. The presence of Ca^{2+} deprotonates sulfinpyrazone at the C(4) and C(4′) positions providing the capability of forming strong hydrogen bonds between O(6) and O(6′). In addition to this, the coordination with calcium through sulfinyl O atoms converts this compound into an active species. The two crystallographically independent molecules exist in two significantly different molecular conformations, indicating that the molecules are flexible and can easily undergo a conformational change as a result of the variation of the intermolecular interactions. The inherent conformational flexibility and cation-induced deprotonated state of sulfinpyrazone make this molecule a suitable species for ligand action. This property of sulfinpyrazone may be responsible for its uricosuric effect.

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The Structure of Cyclonebularine Derivatives

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Abstract. (I) 7,8-Dihydro-2′,3′-*O*-isopropylidene-N^7-(*p*-toluenesulfonyl)-8(*R*),5′-*O*-cyclonebularine, $C_{20}H_{22}N_4O_6S$, M_r = 446·5, triclinic, $P1$, a = 11·069 (1), b = 13·087 (1), c = 8·741 (5) Å, α = 99·31 (1), β = 102·16 (2), γ = 109·81 (1)°, U = 1126·6 (7) Å^3, Z = 2, D_x = 1·316 Mg m^{-3}, λ(Cu $K\alpha_1$) = 1·5405 Å, μ = 1·619 mm^{-1}, $F(000)$ = 468, T = 293 K, final R = 0·035 for 3673 reflexions. (II) N^7-Benzoyl-7,8-dihydro-2′,3′-*O*-isopropylidene-8(*R*),5′-*O*-cyclonebularine, $C_{20}H_{20}N_4O_5$, M_r = 396·4, monoclinic, $P2_1$, a = 11·880 (1), b = 7·603 (1), c = 10·626 (1) Å, β = 102·16 (2)°, U = 958·9 (2) Å^3, Z = 2, D_x = 1·373 Mg m^{-3}, λ(Cu $K\alpha_1$) = 1·5405 Å, μ = 0·850 mm^{-1}, $F(000)$ = 416, T = 293 K, final R = 0·058 for 1498 reflexions. (III) N^7-Acetyl-7,8-dihydro-2′,3′-*O*-isopropylidene-8(*R*),5′-*O*-cyclonebularine, $C_{15}H_{18}N_4O_5$, M_r = 334·3, orthorhombic, $P2_12_12_1$, a = 10·194 (1), b = 18·389 (1), c = 8·400 (4) Å, U = 1574·6 (9) Å^3, Z = 4, D_x = 1·410 Mg m^{-3}, λ(Cu $K\alpha_1$) = 1·5405 Å, μ = 0·918 mm^{-1}, $F(000)$ = 704, T = 293 K, final R = 0·043 for 1337 reflexions. There is substantial difference in the conformations of the *p*-toluoyl groups in the two independent molecules of (I). The 8(*R*)-configuration is observed in all three compounds.

Introduction. In the course of our work on the synthetic chemistry of nucleosides, we obtained a novel type of nebularine (9-β-D-ribofuranosylpurine): N(7)-substituted [*p*-toluoyl (I), benzoyl (II) and acetyl (III)] 7,8-dihydro-8,5′-cyclonebularines

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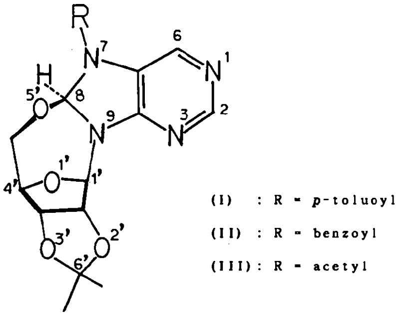
(Hayakawa, Ashizawa, Tanaka, Miyasaka & Yamaguchi, 1989). This paper describes the X-ray structure analysis of these three cyclonebularine derivatives containing the new ring system.



Experimental. Preparation and physical properties of all three compounds are given in Hayakawa *et al.* (1989). Details of data collection and refinement are listed in Table 1. Intensity data collected with a Rigaku AFC5 diffractometer; graphite-monochromated Cu $K\alpha_1$ radiation; θ–2θ scan method; $(1·3 + 0·41\tan\theta)°$ scan width; intensities corrected for Lorentz and polarization factors, absorption correction not applied. Structure solved using the program package *SAPI*85 (Yao, Zheng, Qian, Han, Gu & Fan, 1985) version of *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980).

The refinement was carried out by the full-matrix least-squares method with anisotropic thermal parameters for nonhydrogen atoms; the function minimized was $\sum w[|(|F_o|)^2 - (|F_c|)^2|]^2$ with $w = 1/[\sigma^2(F_o) + 0·02(F_o)^2]$, $\sigma(F_o)$ determined from counting statistics; all H atoms were located from the difference map and theoretical calculations, the initial thermal parameters were set to the equivalent isotropic thermal parameters of bonded atoms. All calculations were performed using a PANAFACOM computer with *RCRYSTAN* (Rigaku Corp., Tokyo, Japan) X-ray analysis program system. The atomic scattering factors were those from *International Tables for X-ray Crystallography* (1974).

Discussion. Final atomic parameters for compounds (I), (II) and (III) are listed in Table 2. The selected bond lengths and angles are listed in Table 3. Fig. 1 shows *ORTEP* drawings (Johnson, 1965) of the molecules (I*A*), (I*B*), (II) and (III). Fig. 2 gives stereoviews of the crystal structures.*

Table 1. *Details of data collection and structure refinement*

	(I)	(II)	(III)
Data collection			
Crystal size (mm)	0·20 × 0·15 × 0·45	0·20 × 0·20 × 0·40	0·40 × 0·20 × 0·50
Cell-parameter determination: No.; θ range (°)	20; 58–61	20; 56–61	20; 54–60
Scan speed (°min^{-1})	8·0	16·0	16·0
Max. $(\sin\theta)/\lambda$(Å^{-1})	0·56	0·56	0·56
Range *h*	−12, 12	−13, 13	11
k	−15, 15	8	20
l	10	11	9
Standard reflexions No.; interval (ref.)	3; 200	3; 150	3;150
No. of reflexions	4210	1689	1424
independent	3843	1557	1372
used for LS	3673[$F > 3\sigma(F)$]	1498 [$F > 3\sigma(F)$]	1337[$F > \sigma(F)$]
Merging *R* for No. of	0·018	0·008	–
equivalent reflexions	285	91	–
Refinement			
R	0·035	0·058	0·043
wR	0·050	0·081	0·051
*G**	1·661	2·876	1·497
$(\Delta/\sigma)_{\max}$	0·69	0·18	0·38
Max. heights in final Fourier map (e Å^{-3})	0·45	0·40	0·32

$*G = \sum w\{[|(|F_o|)^2 - (|F_c|)^2|)]^2/(N_r - N_v)\}^{1/2}$.

Table 2. *Atomic coordinates and equivalent isotropic thermal parameters*

$$B_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j B_{ij}\alpha_i^*\alpha_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	B_{eq}(Å^2)
(I)				
N(1*A*)	−0·2049 (4)	0·7718 (4)	0·0520 (6)	5·64 (19)
C(2*A*)	−0·1757 (6)	0·8659 (5)	0·0056 (7)	6·11 (22)
N(3*A*)	−0·0582 (4)	0·9564 (3)	0·0544 (5)	5·39 (17)
C(4*A*)	0·0358 (4)	0·9427 (3)	0·1617 (5)	4·52 (17)
C(5*A*)	0·0168 (4)	0·8477 (3)	0·2204 (6)	4·30 (17)
C(6*A*)	−0·1049 (5)	0·7623 (4)	0·1641 (6)	4·74 (18)
N(7*A*)	0·1377 (4)	0·8688 (3)	0·3389 (5)	4·38 (16)
C(8*A*)	0·2303 (5)	0·9838 (4)	0·3593 (7)	4·46 (19)
N(9*A*)	0·1636 (4)	1·0193 (3)	0·2325 (4)	4·61 (16)
C(10*A*)	0·2053 (5)	1·1371 (4)	0·2291 (6)	5·03 (19)
C(11*A*)	0·1350 (5)	1·1975 (4)	0·3178 (7)	5·07 (19)
C(12*A*)	0·2398 (6)	1·2667 (4)	0·4800 (7)	5·62 (20)
C(13*A*)	0·3576 (5)	1·2342 (4)	0·4802 (8)	5·62 (21)
O(14*A*)	0·3442 (3)	1·1921 (3)	0·3117 (5)	5·96 (17)
C(15*A*)	0·3655 (5)	1·1473 (4)	0·5723 (8)	5·32 (24)
O(16*A*)	0·2471 (4)	1·0471 (3)	0·5148 (4)	5·06 (16)
O(17*A*)	0·1122 (4)	1·2783 (3)	0·2367 (5)	6·84 (18)
C(18*A*)	0·1653 (6)	1·3847 (4)	0·3517 (9)	6·68 (23)
O(19*A*)	0·2737 (4)	1·3802 (3)	0·4674 (5)	6·94 (18)
C(20*A*)	0·0605 (11)	1·4012 (8)	0·4265 (17)	10·24 (42)
C(21*A*)	0·2238 (10)	1·4745 (7)	0·2703 (14)	9·29 (36)
S(22*A*)	0·1985 (1)	0·7707 (1)	0·3642 (2)	4·72 (12)
O(23*A*)	0·0853 (4)	0·6734 (3)	0·3489 (5)	5·94 (17)
O(24*A*)	0·3112 (4)	0·8200 (3)	0·5017 (4)	5·79 (17)
C(25*A*)	0·2577 (4)	0·7457 (4)	0·1924 (6)	4·47 (19)
C(26*A*)	0·3926 (5)	0·7964 (5)	0·2079 (7)	5·20 (20)
C(27*A*)	0·4401 (6)	0·7746 (5)	0·0767 (7)	6·14 (22)
C(28*A*)	0·3521 (6)	0·7020 (5)	−0·0704 (7)	6·15 (23)
C(29*A*)	0·2176 (6)	0·6535 (5)	−0·0825 (7)	5·92 (22)
C(30*A*)	0·1694 (5)	0·6746 (4)	0·0481 (6)	5·04 (19)
C(31*A*)	0·4061 (10)	0·6811 (9)	−0·2093 (9)	8·69 (35)
N(1*B*)	1·2150 (4)	0·0260 (4)	0·8669 (5)	5·75 (19)
C(2*B*)	1·2070 (5)	−0·0764 (5)	0·8499 (7)	5·75 (21)
N(3*B*)	1·1084 (4)	−0·1720 (3)	0·7545 (5)	5·59 (18)
C(4*B*)	1·0078 (4)	−0·1544 (4)	0·6678 (5)	4·62 (17)
C(5*B*)	1·0015 (5)	−0·0480 (4)	0·6800 (6)	4·70 (18)
C(6*B*)	1·1082 (5)	0·0419 (5)	0·7799 (7)	5·48 (21)
N(7*B*)	0·8771 (4)	−0·0657 (3)	0·5730 (5)	5·14 (17)
C(8*B*)	0·7975 (4)	−0·1872 (4)	0·5067 (6)	4·72 (18)
N(9*B*)	0·8976 (3)	−0·2332 (3)	0·5562 (5)	4·76 (16)
C(10*B*)	0·8581 (5)	−0·3549 (4)	0·5428 (6)	5·01 (19)
C(11*B*)	0·8318 (5)	−0·3835 (4)	0·6971 (7)	5·20 (19)
C(12*B*)	0·6782 (5)	−0·4352 (4)	0·6558 (7)	5·40 (20)
C(13*B*)	0·6276 (5)	−0·4240 (4)	0·4864 (7)	5·30 (20)
O(14*B*)	0·7386 (3)	−0·4130 (3)	0·4177 (4)	5·59 (16)

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* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters and deviations of the atoms from least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52314 (26 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2 (*cont.*)

	x	*y*	*z*	B_{eq}(Å^2)
C(15*B*)	0·5868 (4)	−0·3253 (4)	0·4791 (7)	5·28 (19)
O(16*B*)	0·6919 (3)	−0·2208 (2)	0·5780 (4)	4·80 (15)
O(17*B*)	0·8734 (4)	−0·4717 (4)	0·7241 (7)	7·94 (21)
C(18*B*)	0·7644 (6)	−0·5631 (4)	0·7348 (9)	6·85 (24)
O(19*B*)	0·6474 (3)	−0·5498 (3)	0·6524 (6)	6·76 (18)
C(20*B*)	0·7688 (14)	−0·6700 (9)	0·6527 (23)	12·80 (59)
C(21*B*)	0·7688 (13)	−0·5529 (10)	0·9118 (13)	11·21 (46)
S(22*B*)	0·8138 (1)	0·0298 (1)	0·5581 (1)	5·57 (12)
O(23*B*)	0·9256 (4)	0·1294 (3)	0·5687 (6)	7·07 (19)
O(24*B*)	0·7060 (4)	−0·0197 (4)	0·4104 (5)	6·94 (19)
C(25*B*)	0·7508 (5)	0·0521 (4)	0·7179 (6)	5·07 (19)
C(26*B*)	0·6155 (5)	−0·0016 (5)	0·6996 (8)	5·86 (22)
C(27*B*)	0·5665 (6)	0·0203 (6)	0·8266 (9)	6·78 (25)
C(28*B*)	0·6471 (6)	0·0934 (5)	0·9732 (8)	6·45 (23)
C(29*B*)	0·7838 (7)	0·1459 (6)	0·9905 (9)	6·69 (24)
C(30*B*)	0·8356 (6)	0·1263 (5)	0·8634 (8)	6·02 (22)
C(31*B*)	0·5881 (11)	0·1160 (11)	1·1116 (11)	9·32 (39)
(II)				
N(1)	−0·1411 (5)	0·0509 (9)	1·1818 (5)	6·03 (21)
C(2)	−0·2169 (5)	0·0138 (9)	1·0901 (5)	5·54 (22)
N(3)	−0·2020 (3)	−0·0241 (8)	0·9695 (4)	5·00 (19)
C(4)	−0·0948 (3)	−0·0170 (8)	0·9417 (4)	4·02 (19)
C(5)	−0·0058 (4)	0·0209 (8)	1·0279 (4)	4·15 (19)
C(6)	−0·0305 (5)	0·0537 (8)	1·1480 (5)	4·94 (21)
N(7)	0·0941 (3)	0·0151 (7)	0·9603 (3)	4·26 (18)
C(8)	0·0652 (4)	−0·0028 (8)	0·8253 (4)	3·83 (19)
N(9)	−0·0533 (2)	−0·0503 (7)	0·8251 (3)	3·86 (18)
C(10)	−0·1244 (4)	−0·0502 (9)	0·7100 (4)	4·16 (19)
C(11)	−0·1864 (4)	0·1247 (9)	0·6885 (5)	4·50 (20)
C(12)	−0·1148 (4)	0·2249 (9)	0·5979 (5)	4·35 (20)
C(13)	−0·0196 (4)	0·1029 (9)	0·5657 (5)	4·51 (20)
O(14)	−0·0552 (2)	−0·0707 (6)	0·6062 (3)	4·70 (18)
C(15)	0·0913 (4)	0·1481 (9)	0·6334 (4)	4·56 (20)
O(16)	0·0795 (2)	0·1624 (0)	0·7676 (3)	4·06 (17)
O(17)	−0·2883 (3)	0·0878 (9)	0·6184 (4)	6·56 (20)
C(18)	−0·2983 (4)	0·2170 (12)	0·5220 (5)	5·82 (23)
O(19)	−0·1868 (2)	0·2529 (8)	0·4889 (3)	5·39 (18)
C(20)	−0·3566 (7)	0·1351 (18)	0·4048 (9)	8·58 (35)
C(21)	−0·3529 (7)	0·3808 (16)	0·5669 (9)	8·90 (35)
C(22)	0·2004 (4)	−0·0025 (9)	1·0194 (5)	5·03 (20)
O(23)	0·2065 (3)	−0·0036 (10)	1·1336 (3)	7·11 (21)
C(24)	0·3032 (4)	−0·0157 (9)	0·9436 (4)	4·69 (20)
C(25)	0·3237 (4)	0·0910 (9)	0·8407 (5)	4·99 (21)
C(26)	0·4272 (5)	0·0785 (12)	0·7850 (6)	6·01 (23)
C(27)	0·5071 (5)	−0·0419 (13)	0·8281 (7)	6·97 (27)
C(28)	0·4856 (5)	−0·1475 (13)	0·9270 (8)	6·94 (27)
C(29)	0·2848 (4)	−0·1362 (10)	0·9882 (6)	5·89 (23)
(III)				
N(1)	0·0356 (3)	0·4972 (2)	0·4384 (5)	5·62 (23)
C(2)	0·0978 (4)	0·5583 (3)	0·4165 (7)	5·73 (25)
N(3)	0·2283 (3)	0·5692 (2)	0·3899 (5)	5·01 (22)
C(4)	0·2932 (3)	0·5075 (2)	0·3881 (5)	3·60 (22)
C(5)	0·2384 (3)	0·4385 (2)	0·4105 (5)	3·54 (22)
C(6)	0·1061 (3)	0·4348 (2)	0·4368 (5)	4·37 (23)
N(7)	0·3389 (2)	0·3879 (1)	0·4000 (4)	3·77 (21)
C(8)	0·4645 (3)	0·4248 (2)	0·3882 (5)	3·53 (21)
N(9)	0·4250 (2)	0·4993 (1)	0·3624 (4)	3·65 (21)
C(10)	0·5221 (3)	0·5579 (2)	0·3523 (5)	3·75 (22)
C(11)	0·5349 (3)	0·6002 (2)	0·5069 (5)	3·25 (21)
C(12)	0·6496 (3)	0·5644 (2)	0·5934 (5)	3·36 (21)
C(13)	0·7017 (3)	0·5071 (2)	0·4794 (5)	3·92 (22)
O(14)	0·6452 (2)	0·5264 (1)	0·3260 (3)	4·23 (21)
C(15)	0·6704 (3)	0·4296 (2)	0·5208 (7)	4·40 (22)
O(16)	0·5307 (2)	0·4162 (1)	0·5343 (3)	3·70 (20)
O(17)	0·5807 (2)	0·6711 (1)	0·4694 (3)	4·53 (20)
C(18)	0·6869 (4)	0·6884 (2)	0·5747 (5)	4·20 (22)
O(19)	0·7450 (2)	0·6209 (1)	0·6113 (4)	4·95 (21)
C(20)	0·7833 (6)	0·7346 (3)	0·4840 (9)	6·58 (27)
C(21)	0·6361 (7)	0·7240 (3)	0·7224 (7)	6·34 (26)
C(22)	0·3230 (4)	0·3130 (2)	0·3993 (5)	4·27 (22)
O(23)	0·2137 (3)	0·2879 (1)	0·4181 (4)	5·77 (21)
C(24)	0·4431 (5)	0·2679 (3)	0·3778 (9)	5·74 (25)

Two independent molecules (I*A* and I*B*) are included in an asymmetric unit of (I). The *exo* and *endo* conformations for (I*A*) and (I*B*), respectively, are observed at the *p*-toluoyl group. The C(5)—N(7)—S(22)—C(25) torsion angles are 71·84 (I*A*) and −76·34° (I*B*).

Table 3. *Selected bond lengths* (Å) *and angles* (°)

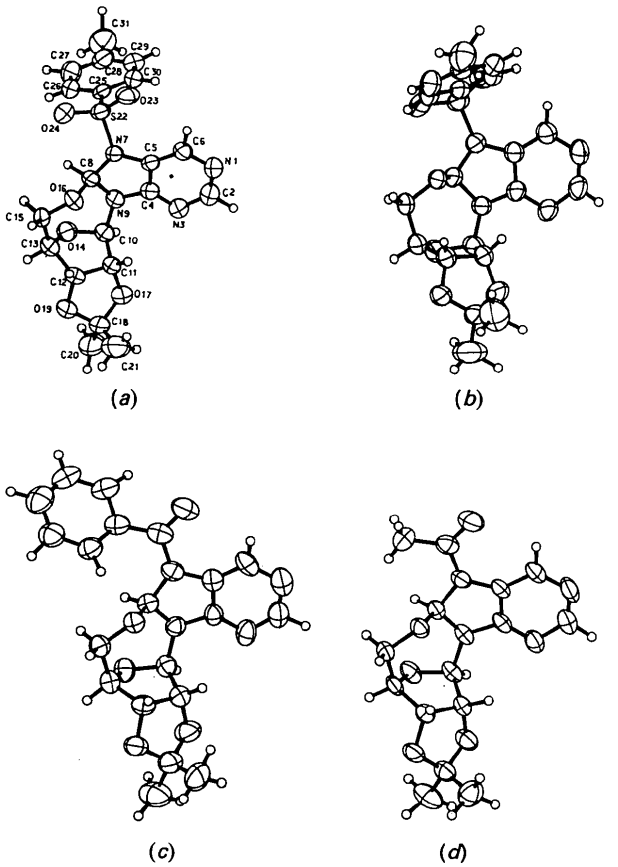
	I*A*	I*B*	II	III
N(1)—C(2)	1·316 (9)	1·295 (10)	1·329 (8)	1·304 (7)
C(2)—N(3)	1·335 (7)	1·344 (6)	1·332 (8)	1·365 (6)
N(3)—C(4)	1·328 (7)	1·320 (7)	1·320 (6)	1·314 (5)
C(4)—C(5)	1·388 (8)	1·406 (8)	1·400 (7)	1·399 (6)
C(5)—C(6)	1·352 (6)	1·354 (6)	1·345 (8)	1·369 (5)
C(6)—N(1)	1·370 (8)	1·362 (9)	1·377 (9)	1·353 (6)
C(5)—N(7)	1·419 (6)	1·412 (7)	1·413 (7)	1·388 (5)
N(7)—C(8)	1·463 (6)	1·475 (6)	1·468 (6)	1·452 (5)
C(8)—N(9)	1·429 (8)	1·454 (8)	1·453 (6)	1·445 (5)
N(9)—C(4)	1·364 (5)	1·351 (5)	1·376 (6)	1·370 (4)
N(9)—C(10)	1·459 (7)	1·478 (7)	1·458 (6)	1·464 (5)
C(10)—C(11)	1·518 (9)	1·517 (9)	1·532 (9)	1·520 (6)
C(11)—C(12)	1·535 (7)	1·537 (7)	1·517 (8)	1·525 (5)
C(12)—C(13)	1·503 (10)	1·518 (9)	1·513 (8)	1·520 (6)
C(13)—O(14)	1·444 (8)	1·452 (8)	1·457 (8)	1·454 (5)
O(14)—C(10)	1·420 (6)	1·401 (6)	1·411 (6)	1·400 (5)
C(13)—C(15)	1·510 (10)	1·512 (10)	1·514 (7)	1·501 (6)
C(15)—O(16)	1·426 (6)	1·444 (5)	1·442 (6)	1·449 (5)
O(16)—C(8)	1·411 (8)	1·412 (7)	1·411 (7)	1·409 (5)
C(11)—O(17)	1·426 (8)	1·415 (9)	1·423 (7)	1·421 (5)
O(17)—C(18)	1·428 (7)	1·415 (8)	1·420 (10)	1·433 (5)
C(18)—O(19)	1·422 (9)	1·425 (9)	1·410 (7)	1·410 (5)
O(19)—C(12)	1·433 (7)	1·414 (7)	1·427 (6)	1·431 (5)
N(1)—C(2)—N(3)	128·4 (6)	129·3 (6)	129·6 (5)	128·6 (4)
C(2)—N(3)—C(4)	112·3 (5)	112·5 (5)	111·9 (4)	111·4 (3)
N(3)—C(4)—C(5)	124·5 (4)	123·6 (3)	124·9 (4)	125·5 (3)
C(4)—C(5)—C(6)	118·2 (5)	117·7 (5)	117·9 (5)	117·3 (3)
C(5)—C(6)—N(1)	119·5 (5)	119·4 (6)	119·5 (5)	118·9 (4)
C(6)—N(1)—C(2)	116·9 (4)	117·0 (4)	115·8 (5)	118·1 (3)
C(5)—C(4)—N(9)	109·8 (4)	110·1 (4)	109·6 (4)	108·2 (3)
C(4)—N(9)—C(8)	110·3 (4)	110·7 (4)	109·7 (3)	110·7 (3)
N(9)—C(8)—N(7)	103·3 (3)	101·2 (3)	102·2 (3)	101·9 (2)
C(8)—N(7)—C(5)	108·4 (4)	109·9 (4)	109·3 (3)	110·0 (3)
C(8)—N(9)—C(10)	121·9 (3)	120·7 (3)	121·9 (3)	121·1 (2)
N(9)—C(10)—C(11)	112·5 (4)	111·2 (4)	112·5 (4)	112·6 (3)
C(10)—C(11)—C(12)	104·6 (4)	104·0 (4)	104·5 (4)	104·5 (3)
C(11)—C(12)—C(13)	105·1 (5)	105·3 (5)	106·2 (5)	105·5 (3)
C(12)—C(13)—O(14)	105·0 (4)	104·4 (4)	105·0 (4)	104·5 (3)
C(13)—O(14)—C(10)	107·9 (4)	108·0 (4)	108·5 (4)	108·3 (3)
O(14)—C(10)—N(9)	108·1 (4)	108·6 (4)	108·6 (3)	108·1 (3)
C(12)—C(13)—C(15)	114·6 (5)	114·9 (5)	113·3 (5)	115·9 (3)
C(13)—C(15)—C(16)	112·2 (4)	111·9 (4)	111·6 (4)	112·8 (3)
C(15)—C(16)—C(8)	113·7 (4)	110·8 (4)	112·.3 (3)	112·5 (3)
C(16)—C(8)—N(9)	112·8 (5)	112·3 (4)	110·8 (4)	111·6 (3)
O(14)—C(13)—C(15)	110·4 (5)	110·2 (5)	108·8 (4)	110·6 (3)
C(11)—O(17)—C(18)	108·6 (4)	109·7 (5)	106·5 (5)	108·3 (3)
O(17)—C(18)—O(19)	103·9 (5)	105·2 (5)	105·2 (4)	104·8 (3)
C(18)—O(19)—C(12)	108·3 (4)	109·4 (3)	107·8 (4)	109·3 (3)
O(19)—C(12)—C(11)	103·5 (4)	104·2 (5)	104·8 (4)	104·8 (3)
C(12)—C(11)—O(17)	105·0 (4)	105·1 (4)	104·7 (4)	104·5 (2)

In all four molecules [(I*A*), (I*B*), (II) and (III)], the geometries of the purine and the fused furan-dioxolane group are almost consistent with each other. The purine rings are closely planar, with maximum displacement of 0.099 (I*A*), 0·109 (I*B*), 0·135 (II) and 0·096 (III) Å out of the least-squares plane. The rather large value is due to the sp^3 character of C(8) compared with nebularine (Takeda, Ohashi & Sasada, 1974) and cordycepin (Radwan & Wilson, 1980).

The furanose ring puckering is O(1′)-*exo*, which is displaced by 0·452 (I*A*), 0·445 (I*B*), 0·433 (II) and 0·459 Å (III) from the least-squares plane through the remaining four atoms. The dioxolane ring is puckered C(6′)-*endo*, with displacement of 0·449 (I*A*), 0·342 (I*B*), 0·447 (II) and 0·391 Å (III).

A closer examination seen in 2′,3′-*o*-isopropylideneadenosine shows the C(3′)-*endo* (molecule 1) and C(3′)-*exo*,C(4′)-*endo* twist (molecule 2) for the furanose ring and C(6′)-*endo*,O(2′)-*exo* (molecule 1) and C(3′)-*endo*,O(3′)-*exo* twist (molecule 2) for the dioxolane ring in the fused furan-dioxolane group (two molecules are included in an asymmetric unit) (Spring, Rohrer & Sundaralingam, 1978). The difference between cyclonebularines and this compound are attributed to the modification in which the furanose ring is cyclized at the C(1′) and C(4′) atoms in cyclonebularines in order to constrain the conformational flexibility of the fused furan-dioxolane group. The dihedral angles between furanose and dioxolane rings are 114·8 (I*A*), 115·0 (I*B*), 114·4 (II) and 114·3° (III).

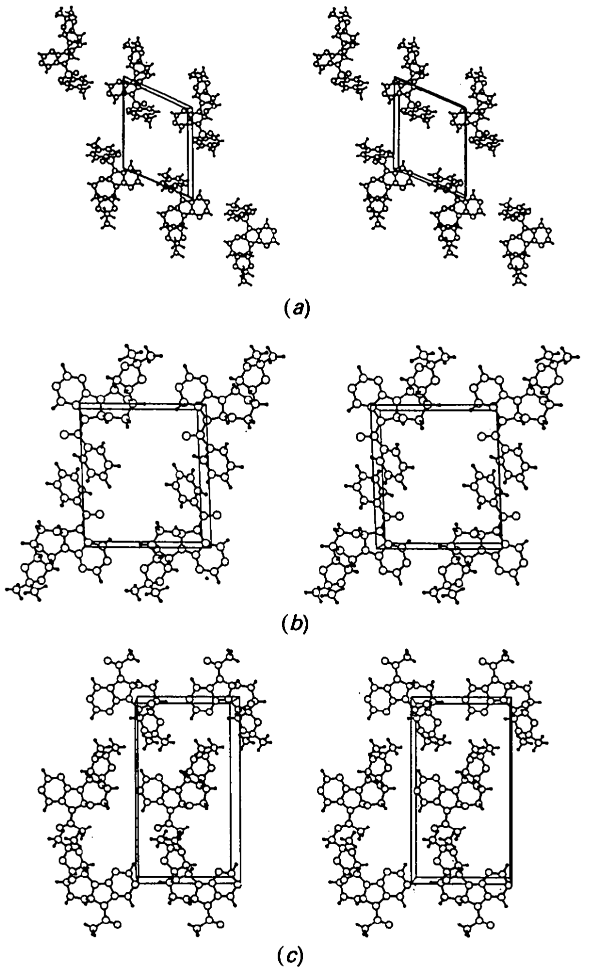
In the seven-membered rings which link up with the purine and fused furan-dioxolane groups, the O(5′)-*endo* conformation and C(8)-*R* configuration are observed in all three compounds. Intermolecular hydrogen bonds and unusual short non-bonding contacts are not observed in all three crystals.



(*a*) (*b*)

(*c*) (*d*)

Fig. 1. *ORTEP* drawings (Johnson, 1965) of the molecules (*a*) (I*A*), (*b*) (I*B*), (*c*) (II) and (*d*) (III). Thermal ellipsoids are drawn at the 50% probability level while isotropic hydrogen thermal parameters are represented by spheres of arbitrary size. Numbers given for the atoms (*a*) are independent of those in the text and conform to those in Tables 2 and 3.



(*a*)

(*b*)

(*c*)

Fig. 2. Stereoviews of the crystal structures of (*a*) (I) shown approximately along the *b* axis, (*b*) (II) along the *c* axis, and (*c*) (III) along the *b* axis.

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