Pd_2S_2 plane have the *anti* conformation. The Pd···Pd length of 3·505 (4) Å seems too long to be assigned as any direct metal–metal interaction. The Pd—S_t (S_t = terminally bound S) bond lengths of 2·337 (6) and 2·336 (7) Å are slightly longer than the Pd—S bond lengths of 2·323 (3) and 2·312 (3) Å for $[Pd(edt)_2]^{2-}$ (edt = ethane-1,2-dithiolate; Snyder, Rao & Holm, 1986). The Pd—S_b (S_b = bridging S) bond lengths of 2·346 (6) and 2·344 (6) Å are also longer than those found in $[Pd_8(S\text{-}n\text{Pr})_{16}]$ (S-*n*Pr = *n*-propanethiolate; Higgins & Suggs, 1988). The bond length order Pd—S_b > Pd—S_t and angle order S_t—Pd—S_t > S_b—Pd—S_b hold in this case, too (Watson, Rao, Dorfman & Holm, 1985).

In the complex anion of (2), the Pt atom is at a center of symmetry. The Pt—S bond lengths of 2·342 (2) and 2·328 (2) Å compare with Pt—S_t bond lengths of 2·317 (5) and 2·342 (5) Å for *cis*-$[(PMePh_2)Pt(SCH_2Ph)(\mu\text{-}SCH_2Ph)]_2$ (Bird, Siriwardane, Lai & Shaver, 1982). The S(1)—Pt—S(2) angle, where the pendant phenyls from S(1) and S(2) are on the same side of the coordination plane, is smaller than 90° [(87·58 (7)°], while the S(1)—Pt—S(2) ($-x$, $-y$, $-z$) angle, where two phenyl groups from S(1) and S(2) ($-x$, $-y$, $-z$) are on the opposite side of the coordination plane, is larger than 90° [92·42 (7)°].

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Structure of Barium α-D-Ribofuranose-5-phosphate Pentahemihydrate: a Reinvestigation

By Anna E. Kozioł

Department of Chemistry, Maria Curie-Skłodowska University, 20-031 *Lublin, Poland*

and Tadeusz Lis

Institute of Chemistry, University, 50-383 *Wrocław, Poland*

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Abstract. $Ba^{2+}.C_5H_9O_8P^{2-}.5\cdot5H_2O$, $M_r = 464\cdot52$, monoclinic, $C2$, $a = 15\cdot469$ (9), $b = 8\cdot622$ (5), $c = 12\cdot865$ (8) Å, $\beta = 118\cdot33$ (5)°, $V = 1510$ (2) Å^3, $Z = 4$, $D_m = 2\cdot047$, $D_x = 2\cdot043$ (2) g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 28\cdot8$ cm^{-1}, $F(000) = 916$, $T = 300$ (2) K, $R = 0\cdot030$ for 6055 hkl and $\bar{h}\bar{k}\bar{l}$ non-zero reflections. The P—O_{ester} bond is 1·616 (2) Å. Distortions from tetrahedral geometry of the phosphate group are similar to those observed in other doubly ionized phosphate esters. The conformation of the α-D-ribofuranose ring is ^2E. The torsion angles P—O(5)—C(5)—C(4), O(5)—C(5)—C(4)—O(4) and O(5)—C(5)—C(4)—C(3) are 170·9 (4), −67·9 (4) and 52·6 (4)°, respectively. Each Ba^{2+} cation is surrounded by ten O atoms (one of them is disordered) at distances of 2·730 (4)–3·338 (3) Å.

Introduction. D-Ribose-5-phosphate is an important constituent of nucleic acids. The structure of the D-ribose fragment in many crystals of nucleotides and other compounds is well documented. However, the free D-ribose-5-phosphate anion is described only in an early work (Furberg & Mostad, 1962) in which the structure of its barium salt is presented. The

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structure was solved and refined using photographic X-ray data. Therefore, we decided to reinvestigate this structure to obtain more accurate results.

Experimental. An irregular fragment (approximately 0·35 × 0·45 × 0·5 mm) was chosen from the commercially available compound (Boehringer). D_m measured by flotation in $CHCl_3/CH_2Br_2$. Preliminary examination by rotation and Weissenberg photographs. Syntex $P2_1$ diffractometer with Mo $K\alpha$ radiation was used for lattice parameter determination (15 reflections in the range $24 \leq 2\theta \leq 29°$) and intensity measurements. The full Ewald sphere to $2\theta_{\max} = 70°$ was measured (h ±24, k ±13, l ±19) using the ω–2θ scan mode; 12371 reflections were collected. Intensities of two standard reflections, measured after every 50 reflections, decreased approximately 11% during 16 d of data collection. The data were rescaled on the intensities of the standards, and corrected for Lorentz–polarization effects. The number of water molecules determined analytically by Levene & Jacobs (1911) was five and half, which is consistent with the measured crystal density. Furberg & Mostad (1962) found positions of five water molecules. Therefore, the structure was solved again by direct methods using *SHELXS*86 (Sheldrick, 1986). Absorption corrections following the *DIFABS* (Walker & Stuart, 1983) procedure were applied; min. and max. correction factors to F were 0·878 and 1·211. The symmetry-related reflections, 11172 with $I > 3\sigma(I)$, were averaged after the *DIFABS* corrections to give 6055 unique reflections (Friedel pairs not averaged); $R_{\text{merge}} = 0{\cdot}0208$. The configuration of the ribose residue used in calculations was consistent with that accepted for D-ribose. The O(5*W*) and O(6*W*) water O atoms, refined with site occupation factors of 1, had large thermal vibration (U_{ij} values 0·047–0·578 Å^2) indicating disorder. The occupancy-factor refinement indicated each of these atoms to be disordered over two sites [O(5*WA*)/O(5*WB*): 0·5/0·5 and O(6*WA*)/O(6*WB*): 0·65/0·35]. The H atoms were found from difference Fourier maps, except two of the disordered O(5*W*) and O(6*W*) water molecules which were not located. Full-matrix least-squares refinement on F of positional and anisotropic thermal parameters of non-H atoms (occupancies for the disordered atoms were fixed at previously obtained values), and isotropic temperature factors of H atoms gave final $R = 0{\cdot}0299$ and $wR = 0{\cdot}0367$ [$w = 1{\cdot}2202/\sigma^2(F_o)$ and isotropic extinction parameter $x = 0{\cdot}00164\,(4)$]. The function minimized was $\sum w(|F_o| - |F_c|)^2$. Residual electron density in final difference map was within $-2{\cdot}56$–$3{\cdot}0$ e Å^{-3} around Ba^{2+} ion; max. Δ/σ for ordered non-H-atom parameters was 0·05. Scattering factors for Ba^{2+}, P, O, C and H atoms, with real- and imaginary-dispersion corrections included for all non-H atoms, were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). The refinement was carried out using *SHELX*76 (Sheldrick, 1976). The final atomic parameters are given in Table 1.*

Table 1. *Fractional atomic coordinates* (× 10^4) *and equivalent isotropic temperature factors* (Å^2) *for barium* D-*ribose-5-phosphate* 5·5 H_2O

$$U_{\text{eq}} = [U_{11}(a^*\mathbf{a})^2 + U_{22}(b^*\mathbf{b})^2 + U_{33}(c^*\mathbf{c})^2 + 2(U_{12}a^*b^*\mathbf{ab}\cos\gamma + U_{13}a^*c^*\mathbf{ac}\cos\beta + U_{23}b^*c^*\mathbf{bc}\cos\alpha)]/3.$$

	x	y	z	U_{eq}
Ba	6831·4 (1)	5000	256·2 (1)	0·0248 (1)
P(1)	9000·1 (4)	4987 (2)	7481·1 (5)	0·0153 (2)
O(1)	8639 (2)	5691 (3)	2344 (2)	0·024 (1)
O(2)	7667 (2)	3219 (3)	2447 (2)	0·025 (1)
O(3)	6713 (2)	5840 (3)	2335 (2)	0·024 (1)
O(4)	8923 (2)	6465 (4)	4214 (2)	0·033 (1)
O(5)	8583 (2)	5120 (4)	6070 (2)	0·021 (1)
O(1*P*)	9875 (2)	6081 (3)	8044 (2)	0·024 (1)
O(2*P*)	8178 (2)	5486 (3)	7731 (2)	0·024 (1)
O(3*P*)	9294 (2)	3312 (3)	7767 (2)	0·025 (1)
C(1)	8886 (2)	5205 (4)	3497 (2)	0·021 (1)
C(2)	8072 (2)	4157 (3)	3458 (2)	0·019 (1)
C(3)	7350 (2)	5330 (3)	3512 (2)	0·019 (1)
C(4)	8032 (2)	6615 (4)	4272 (2)	0·022 (1)
C(5)	8246 (3)	6594 (4)	5546 (3)	0·050 (2)
O(1*W*)	8406 (2)	6551 (3)	− 105 (2)	0·029 (1)
O(2*W*)	6177 (4)	7251 (8)	− 1439 (6)	0·107 (5)
O(3*W*)	7295 (3)	3503 (4)	8641 (4)	0·061 (3)
O(4*W*)[a]	5000	6926 (5)	0	0·043 (2)
O(5*WA*)[a]	5110 (5)	4169 (8)	− 1669 (8)	0·055 (4)
O(5*WB*)[a]	4913 (6)	3920 (8)	− 1043 (8)	0·054 (4)
O(6*WA*)[b]	10126 (17)	9128 (23)	4072 (14)	0·249 (25)
O(6*WB*)[c]	9577 (29)	11756 (37)	5281 (46)	0·279 (40)

Site occupation factors: (*a*) 0·5; (*b*) 0·65; (*c*) 0·35.

Discussion. The crystals of the title salt consist of D-ribose 5-phosphate dianions, Ba^{2+} cations, five water molecules coordinated to Ba^{2+} and one water of crystallization molecule. A view showing the configuration and atom-numbering scheme of the dianion is presented in Fig. 1. The bond lengths and angles and some torsion angles are given in Table 2.

The dianion exists as α-D-ribofuranose which is different from the β-D-ribofuranose configuration observed in 5′-phosphoribonucleotides. The conformation of the furanose ring is ^2E [Cremer & Pople (1975) parameters are $Q_2 = 0{\cdot}342\,(4)$ Å and $\varphi_2 = 73{\cdot}8\,(7)°$]. The two endocyclic O(4)—C bond lengths in the ribose ring are comparable, in contrast to values found in ribonucleotides and ribonucleosides, where the O(4)—C(4) distance is longer than that of O(4)—C(1) (*e.g.* Larson, Anderson, Revankar & Robins, 1988; Brown & Bugg, 1980; Kumar, Patil,

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* Lists of structure factors, anisotropic thermal parameters, puckering and asymmetry ring analysis, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54095 (41 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å), *barium coordination distances* (Å), *bond angles* (°) *and selected torsion angles* (°) *in barium* D-*ribose-5-phosphate* 5·5H_2O

P(1)—O(5)	1·616 (2)	Ba—O(1)	2·874 (2)
P(1)—O(1*P*)	1·521 (2)	Ba—O(2)	2·918 (2)
P(1)—O(2*P*)	1·515 (2)	Ba—O(3)	2·860 (2)
P(1)—O(3*P*)	1·507 (3)	Ba—O(1*W*)	3·001 (3)
O(1)—C(1)	1·408 (4)	Ba—O(2*W*)	2·730 (4)
O(2)—C(2)	1·401 (4)	Ba—O(3$W^{\rm i}$)	2·812 (3)
O(3)—C(3)	1·428 (4)	Ba—O(4*W*)	3·163 (2)
O(4)—C(1)	1·410 (4)	Ba—O(5*WA*)	2·735 (7)
O(4)—C(4)	1·420 (4)	Ba—O(5*WB*)	2·785 (8)
O(5)—C(5)	1·417 (5)	Ba—O($1^{\rm ii}$)	2·992 (2)
C(1)—C(2)	1·531 (4)	Ba—O(3$W^{\rm iii}$)	3·338 (3)
C(2)—C(3)	1·534 (4)		
C(3)—C(4)	1·522 (4)		
C(4)—C(5)	1·511 (5)		

O(5)—P(1)—O(1*P*)	106·3 (2)	O(2)—C(2)—C(1)	111·6 (2)
O(5)—P(1)—O(2*P*)	106·9 (1)	O(2)—C(2)—C(3)	114·1 (2)
O(5)—P(1)—O(3*P*)	104·8 (2)	C(1)—C(2)—C(3)	102·4 (2)
O(1*P*)—P(1)—O(2*P*)	111·7 (2)	O(3)—C(3)—C(2)	107·8 (2)
O(1*P*)—P(1)—O(3*P*)	112·4 (1)	O(3)—C(3)—C(4)	112·1 (2)
O(2*P*)—P(1)—O(3*P*)	114·0 (1)	C(2)—C(3)—C(4)	102·2 (2)
C(1)—O(4)—C(4)	111·4 (2)	O(4)—C(4)—C(3)	107·2 (3)
P(1)—O(5)—C(5)	117·3 (3)	O(4)—C(4)—C(5)	109·7 (3)
O(1)—C(1)—O(4)	111·6 (3)	C(3)—C(4)—C(5)	114·6 (3)
O(1)—C(1)—C(2)	109·5 (2)	O(5)—C(5)—C(4)	111·6 (3)
O(4)—C(1)—C(2)	104·7 (2)		

C(1)—O(4)—C(4)—C(3)	−0·2 (7)	O(1*P*)—P(1)—O(5)—C(5)	−60·7 (5)
O(4)—C(4)—C(3)—C(2)	21·2 (7)	O(2*P*)—P(1)—O(5)—C(5)	58·5 (5)
C(4)—C(3)—C(2)—C(1)	−32·5 (8)	O(3*P*)—P(1)—O(5)—C(5)	179·9 (5)
C(3)—C(2)—C(1)—O(4)	33·4 (7)	P(1)—O(5)—C(5)—C(4)	170·9 (4)
C(2)—C(1)—O(4)—C(4)	−21·2 (7)		

Symmetry code: (i) x, y, $z-1$; (ii) $1{\cdot}5-x$, $y-0{\cdot}5$, $-z$; (iii) $1{\cdot}5-x$, $0{\cdot}5+y$, $1-z$.

Table 3. *Probable hydrogen bonds* (Å) *and angles* (°) *in barium* D-*ribose-5-phosphate* 5·5H_2O

O—H···O	O—H	H···O	O···O	O—H···O
O(1)—H(10)···O(1$P^{\rm i}$)	0·97	1·65	2·596 (5)	166
O(2)—H(20)···O(2$P^{\rm ii}$)	0·95	1·71	2·651 (4)	170
O(3)—H(30)···O(3$P^{\rm iii}$)	0·88	1·74	2·606 (4)	165
O(1*W*)—H(1*W*1)···O(2$P^{\rm iv}$)	0·90	1·91	2·790 (4)	164
O(1*W*)—H(1*W*2)···O(1$P^{\rm i}$)	0·91	1·85	2·753 (3)	176
O(2*W*)—H(2*W*1)···O($2^{\rm v}$)	0·96	2·05	2·789 (9)	132
O(2*W*)—H(2*W*2)···O(3$P^{\rm vi}$)	0·74	2·03	2·746 (7)	165
O(3*W*)—H(3*W*1)···O($1^{\rm ii}$)	0·95	2·11	2·800 (4)	128
O(3*W*)—H(3*W*2)···O(2$P^{\rm vii}$)	0·87	1·95	2·770 (6)	156
O(4*W*)—H(4*W*)···O(3$P^{\rm iii}$)	0·81	2·00	2·810 (3)	178
O(5*WA*)—H(5*W*)···O($3^{\rm viii}$)	1·01	1·92	2·910 (8)	165
O(5*WB*)—H(5*W*)···O($3^{\rm viii}$)	1·08	1·92	2·804 (8)	136
O(6*WB*)—H(6*WB*)···O(6$WA^{\rm vii}$)	1·10	2·07	3·09 (6)	152
O(5*WA*)···O(1$P^{\rm ix}$)			2·69 (1)	
O(5*WB*)···O(1$P^{\rm ix}$)			2·70 (1)	
O(5*WA*)···O(6$WA^{\rm x}$)			2·94 (5)	
O(5*WB*)···O(1$W^{\rm x}$)			3·08 (1)	
O(6*WA*)···O($4^{\rm vii}$)			3·02 (5)	
O(6*WA*)···O($4^{\rm i}$)			3·04 (5)	

Symmetry code: (i) $2-x$, y, $1-z$; (ii) $1{\cdot}5-x$, $y-0{\cdot}5$, $1-z$; (iii) $1{\cdot}5-x$, $0{\cdot}5+y$, $1-z$; (iv) x, y, $z-1$; (v) $1{\cdot}5-x$, $0{\cdot}5+y$, $-z$; (vi) $x-0{\cdot}5$, $0{\cdot}5+y$, $z-1$; (vii) x, y, z; (viii) $1-x$, y, $-z$; (ix) $x-0{\cdot}5$, $y-0{\cdot}5$, $z-1$; (x) $1{\cdot}5-x$, $y-0{\cdot}5$, $-z$.

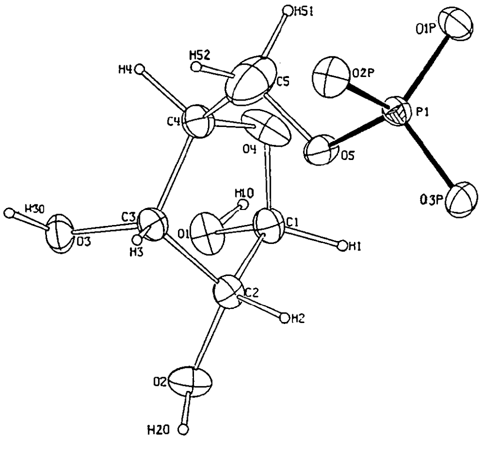

Fig. 1. A perspective view of the D-ribose-5-phosphate dianion showing its configuration and atom-numbering scheme.

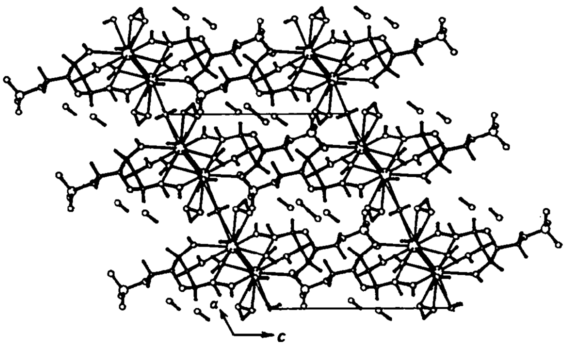

Fig. 2. The molecular packing in the crystal.

Wilson & Leonard, 1989; Singh & Hodgson, 1989). The conformation around the exocyclic C(4)—C(5) bond is *gauche–gauche*, as indicated by the torsion angles O(5)—C(5)—C(4)—C(3) and O(5)—C(5)—C(4)—O(4) [52·6 (4) and −67·9 (4)°]. The orientation of the phosphate group with respect to the sugar residue is defined by the C(4)—C(5)—O(5)—P(1) torsion angle of 170·9 (4)°. The P—O(5) ester bond length [1·616 (2) Å] is similar to those found in doubly ionized D-ribose-5-phosphate moieties (Jeffrey & Sundaralingam, 1986). The distortion of the phosphate group from an idealized tetrahedral geometry is essentially the same as in all doubly ionized organic phosphates (Starynowicz & Lis, 1985), *i.e.* the O(3P) *trans* oriented to atom C(5) forms the smallest of the O—P—$O_{\rm ester}$ bond angles. This gives the O(3P)···O(5) distance of 2·48 Å, while the average of the other five O···O distances within the PO_4 tetrahedron is 2·52 Å.

The packing in the crystal is shown in Fig. 2. The Ba^{2+} ions are ten coordinate, with Ba—O distances between 2·730 (4) and 3·338 (3) Å. The phosphate O atoms do not coordinate to Ba^{2+}, but accept strong hydrogen bonds.

Each ribose residue chelates the cation through three hydroxyl groups; the irregular coordination sphere is completed by seven water molecules, one of them is disordered [the O(5*WA*)···O(5*WB*) distance is 1·01 (1) Å].

The Ba^{2+} ions are linked by the O(4*W*) molecule (lying on the twofold axis) [Ba···Ba; $1 - x$, y, $-z$] and bonded along the 2_1 axis by O(*W*1) and O(*W*3) water molecules [Ba···Ba; $1{\cdot}5 - x$, $y + 0{\cdot}5$, $-z$]; the Ba···Ba separations are 5·38 (1) and 4·96 (1) Å, respectively. The result is a two-dimensional net of Ba cations, parallel to the *xy* plane, with Ba coordination polyhedra sharing vertices or edges.

The hydroxyl and water H atoms are involved in hydrogen bonds. The hydrogen-bonding data are summarized in Table 3. Because some H-atom positions of the disordered water molecules are missing, only the O···O distances may suggest a possibility of hydrogen bonds. The disordered O(*W*6) water molecule is situated about 3·0 Å apart from the other O atoms, hence no strong hydrogen bonding involving the water of crystallization would be expected. This explains the easy loss of part of water from the crystal (Furberg & Mostad, 1962).

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Structure of Hydridotris[3-(*p*-tolyl)pyrazolyl]boratothallium(I)

By George Ferguson* and Michael C. Jennings

Department of Chemistry and Biochemistry, University of Guelph, Guelph, Ontario, Canada N1G 2W1

and Fergus J. Lalor* and Claire Shanahan

Department of Chemistry, University College, Cork, Republic of Ireland

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Abstract. $C_{30}H_{28}BN_6Tl$, $M_r = 687{\cdot}8$, trigonal, $R3c$, $a = 17{\cdot}551$ (4), $c = 31{\cdot}414$ (6) Å, $V = 8380$ (5) Å^3, $Z = 12$, $D_x = 1{\cdot}64$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 58{\cdot}7$ cm^{-1}, $F(000) = 4032$, $T = 294$ K, $R = 0{\cdot}017$ for 1034 unique reflections with $I > 2\sigma(I)$. There are two independent molecules of the complex in the asymmetric unit, both lying on crystallographic threefold axes. The two independent Tl—N bond lengths are 2·568 (4) and 2·587 (5) Å. In one molecule the *p*-tolyl ring is almost coplanar with the pyrazolyl ring to which it is bonded (interplanar angle 1·8°); in the other molecule the corresponding angle is 29·6°. The shortest Tl···Tl intermolecular distance is 3·8636 (4) Å along the threefold axis.

Introduction. Recent work from these and other laboratories has demonstrated amply that the chemical and structural properties of poly(1-pyrazolyl)borato complexes are remarkably sensitive to changes in the nature of the substituent at the 3-position of the pyrazolyl groups (Desmond, Lalor, Ferguson, Ruhl & Parvez, 1983; Trofimenko, Calabrese, Domaille & Thompson, 1989; Trofimenko, Calabrese & Thompson, 1987). In connection with a study of Group VI transition metal complexes containing sterically crowded poly(1-pyrazolyl)borate ligands, we had occasion

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* E-mail addresses: GF CHMFERG@VM.UOGUELPH.CA
FJL STCH8002@IRUCCVAX

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