Table 6. *Bond strengths in* $Li_2SnF_6.2H_2O$

	Sn	Li	H(1)	H(2)	Sum
F(1)	0.68 (×4)†	0.17 (×2)†	0.09 (×2)†	0.06 (×2)	1.00
F(2)	0.64 (×2)†	(×2)* 0.14 (×2)†		0.06	0.98
O		0.18 (×2)†	0.81	0.81	1.98
Sum	4.00	0.98	0.99	0.99	

Bond strengths (s) calculated after Brown & Shannon (1973) using the parameters

	s_0	R_0	N
Sn–F	0.667	1.969	6.3
Li–F	0.5	1.547	4.0
Li–O	1.0	1.378	4.165

in the equation $s=s_0(R/R_0)^{-N}$. Hydrogen bond strengths estimated.

* Multiplicity around anion.
† Multiplicity around cation.

hedron compared with the TiF_6 octahedron and the correspondingly larger distortion in the environment of Li (see Table 5). A bond strength calculation (Table 6) indicates that the hydrogen bonding scheme is probably similar to that in the Ti compound.

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L-α-Glycerylphosphorylethanolamine Monohydrate

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Abstract. $C_5H_{14}O_6NP.H_2O$, monoclinic, space group $P2_1$ with $a=9{\cdot}566$ (5), $b=7{\cdot}324$ (5), $c=7{\cdot}657$ (5) Å, $\beta=106{\cdot}72$ (2)°; $d_{\text{meas}}=1{\cdot}51$, $d_{\text{calc}}=1{\cdot}507$ g cm^{-3} for $Z=2$; μ(Cu $K\alpha$)$=25{\cdot}6$ cm^{-1}. The absolute configuration has been confirmed from the intensities of 710 Bijvoet pairs hkl and $h\bar{k}l$, using the Cu $K\alpha$ anomalous scattering of phosphorus and oxygen atoms. Bond lengths and angles are reported with e.s.d.'s of about 0·004 Å and 0·3°.

Experimental. A suitable crystal was selected from a sample of L-α-glycerylphosphorylethanolamine monohydrate (hereafter GPE.H_2O), which was prepared by Baer & Stancer (1953) and was kindly supplied by Professor Baer of the University of Toronto. In order

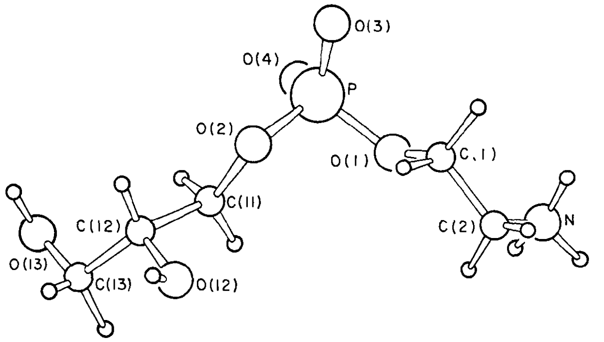

Fig. 1. The atomic nomenclature, conformation, and absolute configuration for the L-α-GPE zwitterion.

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to decrease errors due to X-ray absorption, the plate-like crystal, of dimensions 0·4 × 0·2 × 0·05 mm, was embedded in a spherical bead of epoxy resin of diameter 0·4 mm, and $\mu(\mathrm{Cu}\ K\alpha) \simeq 7\ \mathrm{cm}^{-1}$. The data were measured on a computer-controlled four-circle automatic diffractometer using nickel-filtered Cu *Kα* radiation. The crystal was mounted with *b*, the longest dimension, at an angle of 14·07° from the diffractometer φ axis. Intensities were measured for 1580 reflections with $\sin\theta/\lambda \le 0{\cdot}59\ \text{Å}^{-1}$, using $\theta/2\theta$ scans at a rate of 2°/min and background counts of 20 sec at each scan limit. The data included 710 Bijvoet pairs

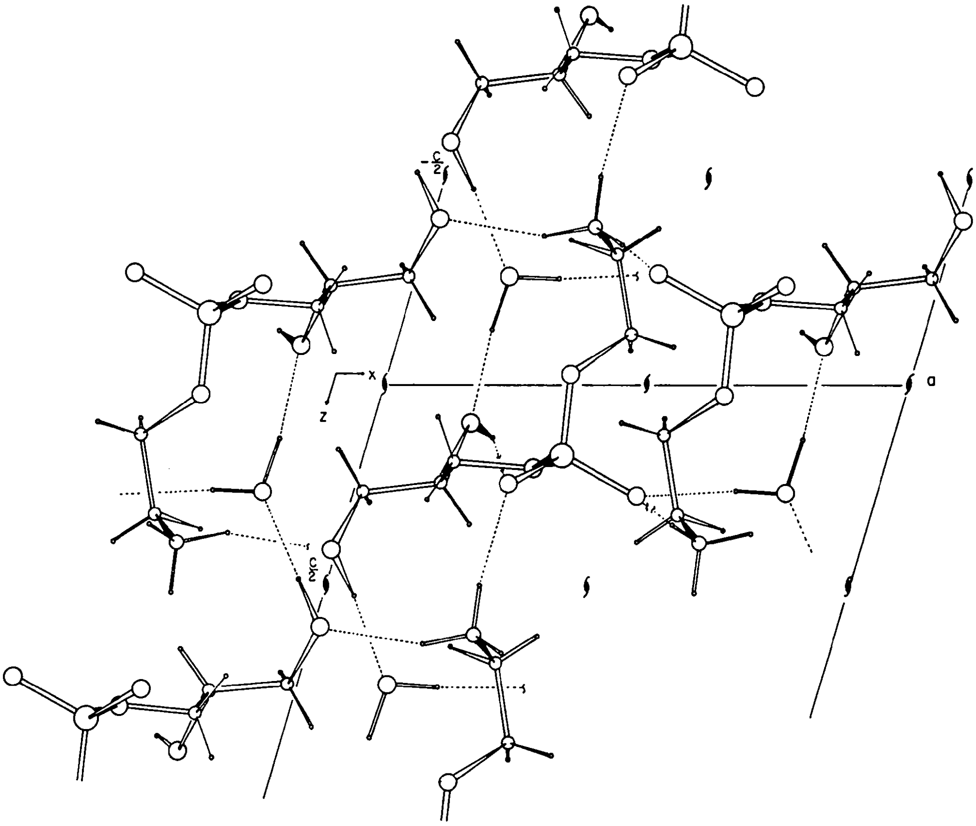

Fig. 2. The crystal structure of L-α-GPE.H_2O in projection down the *b* axis. Hydrogen bonds are shown dotted.

Table 1. *Atomic positional* (× 10^4) *and anisotropic thermal parameters for* L-α-GPE.H_2O

The temperature factor is $T=\exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\right]$. The e.s.d.'s are given in parentheses and refer to the least significant figure in the parameter value.

	x	*y*	*z*	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
N	3124 (3)	4031 (4)	−3871 (3)	0·0083(3)	0·0110 (5)	0·0089 (4)	0·0000 (3)	0·0027 (3)	0·0003 (4)
C(2)	3679 (4)	2174 (5)	−3206 (4)	0·0133 (4)	0·0109 (8)	0·0114 (5)	0·0023 (5)	0·0050 (4)	−0·0003 (4)
C(1)	4428 (4)	2153 (5)	−1219 (4)	0·0104 (4)	0·0145 (7)	0·0119 (6)	0·0026 (5)	0·0049 (4)	0·0010 (5)
O(1)	3463 (2)	2855 (3)	−254 (3)	0·0074 (2)	0·0151 (5)	0·0102 (3)	0·0020 (3)	0·0032 (2)	0·0005 (3)
P	3820·1 (7)	2500	1877·5 (8)	0·00710 (8)	0·0082 (1)	0·0080 (1)	0·0008 (1)	0·00248 (7)	0·0011 (1)
O(3)	5426 (2)	2408 (4)	2726 (2)	0·0079 (2)	0·0170 (4)	0·0131 (4)	0·0001 (3)	0·0006 (2)	0·0028 (4)
O(4)	2940 (3)	3873 (3)	2537 (3)	0·0138 (3)	0·0119 (4)	0·0114 (4)	0·0038 (3)	0·0059 (3)	0·0015 (3)
O(2)	3262 (2)	503 (3)	2094 (3)	0·0083 (2)	0·0092 (4)	0·0217 (5)	0·0011 (3)	0·0072 (3)	0·0033 (4)
C(11)	1749 (3)	111 (4)	1919 (5)	0·0079 (4)	0·0096 (5)	0·0167 (7)	0·0016 (4)	0·0043 (4)	0·0020 (5)
C(12)	1643 (3)	−1868 (4)	2414 (4)	0·0078 (3)	0·0104 (6)	0·0098 (5)	0·0005 (3)	0·0030 (3)	0·0018 (4)
O(12)	1832 (3)	−2950 (3)	963 (3)	0·0147 (3)	0·0105 (5)	0·0151 (4)	0·0035 (3)	0·0066 (3)	0·0025 (3)
C(13)	167 (3)	−2279 (6)	2694 (4)	0·0081 (3)	0·0148 (8)	0·0153 (6)	−0·0017 (4)	0·0039 (4)	−0·0005 (6)
O(13)	−122 (2)	−1269 (4)	4115 (3)	0·0085 (3)	0·0225 (5)	0·0154 (4)	0·0023 (3)	0·0043 (3)	0·0008 (4)
O(*W*)	1788 (3)	−2024 (5)	−2600 (4)	0·0108 (3)	0·040 (1)	0·0156 (5)	0·0026 (5)	0·0032 (3)	0·0033 (6)

Table 1 (*cont.*)

Hydrogen atomic parameters are $\times 10^3$.

	x	y	z
H(1)	218(5)	422(8)	−366 (6)
H(2)	293 (5)	396 (8)	−509 (7)
H(3)	380 (6)	491 (9)	−342 (7)
H(4)	275 (5)	130 (8)	−355 (7)
H(5)	438 (5)	174 (8)	−387 (6)
H(6)	453 (5)	89 (8)	−82 (6)
H(7)	529 (5)	306 (8)	−96 (6)
H(8)	120 (5)	30 (9)	81 (7)
H(9)	138 (5)	88 (8)	281 (6)
H(10)	245 (5)	−198 (7)	349 (7)
H(11)	230 (6)	−410 (8)	130 (8)
H(12)	30 (5)	−350 (9)	289 (6)
H(13)	−55 (5)	−200 (8)	160 (7)
H(14)	55 (5)	−152 (8)	524 (7)
H(15)	172 (5)	−216 (8)	−133 (7)
H(16)	257 (6)	−198 (8)	−256 (6)

(*hkl* and $h\bar{k}l$) and 52 reflections with integrated intensity less than 1·25 $\sigma(I)$. The latter were assigned intensity values of $\sigma(I)/2$.

The phase problem was solved by a combination of Patterson and direct methods. The complete data set (*hkl* and $h\bar{k}l$) was used in full-matrix least-squares refinement of the parameters listed in Table 1. The function minimized was $\sum_{\mathbf{h}}[\Delta F/\sigma(F)]^2$ where $\sigma^2(F)=0{\cdot}1+0{\cdot}001|F|^2$, and $\Delta F=|F_{\text{meas}}|-|F_{\text{calc}}|$. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1968), except that for hydrogen, which was taken from Stewart, Davidson & Simpson (1965). Anomalous scattering factors for phosphorus and oxygen atoms were included ($\Delta f'=0{\cdot}2$, $\Delta f''=0{\cdot}5$ for phosphorus; $\Delta f'=0{\cdot}0$, $\Delta f''=0{\cdot}1$ for oxygen). Independent refinements for enantiomeric crystal structures converged at R values of 0·029 and 0·039 respectively ($R=\sum_{\mathbf{h}}|\Delta F|/\sum|F_{\text{meas}}|$), confirming the absolute configuration (Fig. 1) which was established by Baer & Stancer (1953) from chemical evidence. The differentiation of the enantiomeric structures was enhanced by calculation of $R_{\text{anom}}=\sum_{\mathbf{h}}|\Delta_{\text{meas}}-\Delta_{\text{calc}}|/\sum_{\mathbf{h}}|\Delta_{\text{meas}}|$ where $\Delta=(F_{\mathbf{h}}^2-F_{\bar{\mathbf{h}}}^2)$. This residual had values of 0·58 for the L-structure (Table 1 and Fig. 1) and 1·88 for the D-structure. The observed and calculated (L-isomer) structure amplitudes and Δ-values are listed in Table 2.

Discussion. The conformation of the GPE zwitterion in the crystal structure of GPE.H_2O (Fig. 1), and the significance which this may have in contributing to an understanding of structural relationships in biological membranes have been discussed elsewhere (DeTitta & Craven, 1971; Sundaralingam, 1972). We now report details of the bond lengths and angles (Table 3) and molecular interactions (Fig. 2) in GPE.H_2O.

The bond lengths and angles are similar to those found in α-glycerylphosphorylcholine (Abrahamsson & Pascher, 1966). In particular, the sum of the P–O

Table 2. *Observed and calculated structure amplitudes for* L-α-GPE.H_2O

The columns are k, $10|F_o|$, $10|F_c|$, $10\Delta_o$, $10\Delta_c$. An asterisk appears to the right of the k index for those reflections for which only $F_{h\bar{k}l}$ was measured.

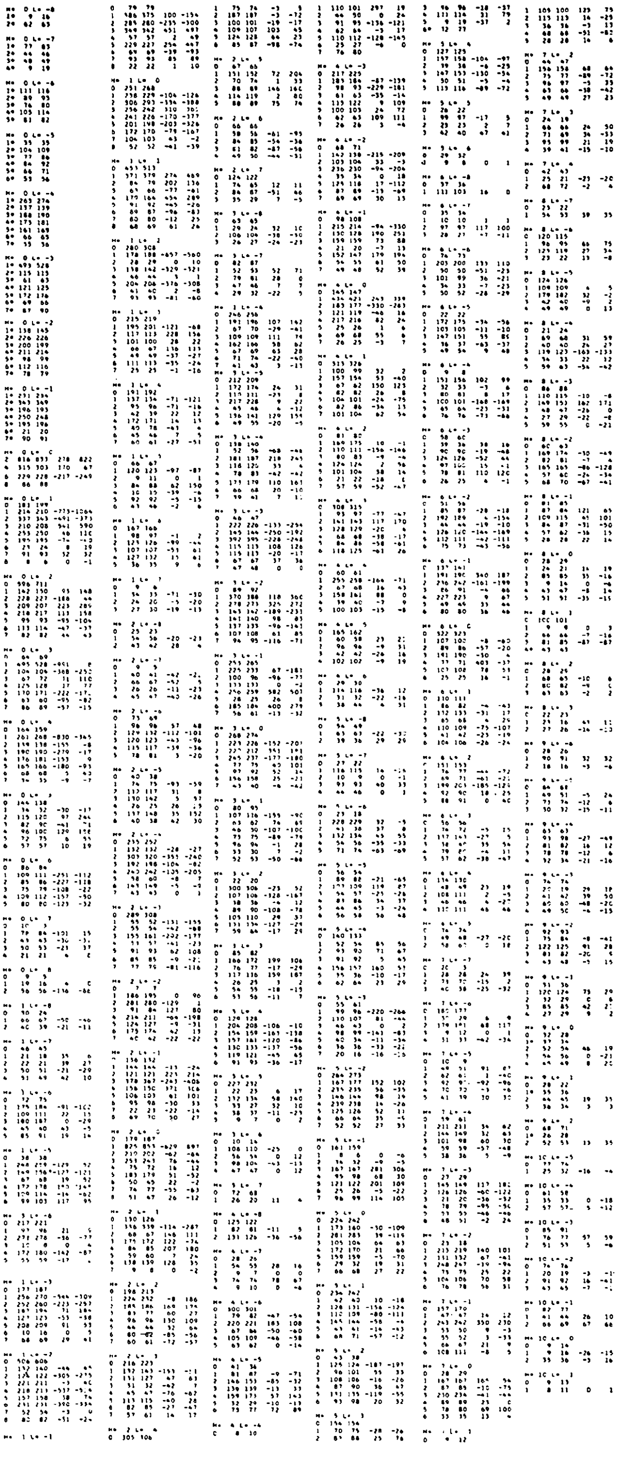

Table 3. *Bond distances and bond angles, with e.s.d.'s, for* L-α-GPE.H_2O

N——C(2)	1·495 (4) Å
C(2)—C(1)	1·483 (5)
C(1)—O(1)	1·433 (4)
P——O(1)	1·590 (2)
P——O(2)	1·582 (2)
P——O(3)	1·486 (2)
P——O(4)	1·489 (3)
O(2)—C(11)	1·443 (4)
C(11)-C(12)	1·508 (4)
C(12)-O(12)	1·418 (4)
C(12)-C(13)	1·517 (5)
C(13)-O(13)	1·407 (4)
N···O(1)	2·827 (3)
N-H	0·90–0·97 (5)
O-H	0·74–1·00 (6)
C-H	0·87–1·06 (5)

N——C(2)—C(1)	112·2 (3)°
C(2)—C(1)—O(1)	109·4 (3)
C(1)—O(1)—P	119·4 (3)
O(1)—P——O(2)	106·2 (1)
O(1)—P——O(3)	110·3 (1)
O(1)—P——O(4)	105·2 (2)
O(2)—P——O(3)	104·4 (1)
O(2)—P——O(4)	110·3 (1)
O(3)—P——O(4)	119·7 (1)
P——O(2)—C(11)	122·3 (3)
O(2)—C(11)-C(12)	107·8 (2)
C(11)-C(12)-O(12)	107·9 (2)
C(11)-C(12)-C(13)	111·0 (3)
O(12)-C(12)-C(13)	109·4 (3)
C(12)-C(13)-O(13)	113·8 (3)

bond lengths, 6·147 (9) Å, in GPE.H_2O is within the range 6·177±0·030 Å which has been observed in 16 accurately determined crystal structures of phosphates (Calleri & Speakman, 1964).

In the crystal structure of GPE.H_2O, there is a three-dimensional network of hydrogen bonds which involves all N–H and O–H donor groups. We do not consider the cationic NH_3^+ group to be intramolecularly hydrogen bonded because, although the intramolecular NH···O distance is short (2·83 Å), the N–H(1)···O angle (86°) is unfavorable. However, the NH_3^+ group forms normal hydrogen bonds with three neighboring zwitterions. As might be expected, these involve both of the electronegative phosphoryl oxygen atoms [N···O distances 2·848 (3) and 2·708 (3) Å]. The third hydrogen bond is with the γ-hydroxyl oxygen atom [N···O(13) distance 2·831 (4) Å]. Each hydroxyl group donates and accepts one hydrogen bond with O···O distances of O(13)H···O(*W*) 2·707 (4) Å, O(12)H···O(4) 2·693 (3) Å, O(*W*)H···O(12) 2·800 (4) Å and O(*W*)H···O(3) 2·728 (4) Å. The water oxygen atom is 0·136 Å out of the plane of the three oxygen atoms with which it is hydrogen bonded. Although the phosphoryl oxygen atoms both accept two hydrogen bonds, the phosphate ester oxygen atoms are not hydrogen bonded. This is consistent with most other crystal structures which contain molecules with phosphodiester linkages (Sundaralingam, 1969).

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