Table 6. Bond strengths in Li₂SnF₆. 2H₂O

	Sn	Li	H(1)	H(2)	Sun
F(1)	0.68 (×4)†	$0.17 (\times 2)^{+}$	0.09 (×2)†	0.06 (×2)	1.00
F(2)	$0.64 (\times 2)^{\dagger}$	$(\times 2)^* 0.14 (\times 2)^{\dagger}$		0.06	0.98
о`́		$0.18(\times 2)^{+}$	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

	<i>S</i> 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=9.566 (5), b=7.324 (5), c=7.657 (5) Å, $\beta=106.72$ (2)°; $d_{meas}=1.51$, $d_{calc}=1.507$ g cm⁻³ for Z=2; $\mu(Cu \ K\alpha)=25.6$ 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 α 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 $L-\alpha$ -glycerylphosphorylethanolamine mono-hydrate (hereafter GPE. H₂O), 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 $L-\alpha$ -GPE zwitterion.

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tion. 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 $\sin \theta/\lambda \le 0.59$ 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. H₂O in projection down the *b* axis. Hydrogen bonds are shown dotted.

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	У	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)
$\tilde{C}(1)$	4428 (4)	2153 (5)	- 1219 (4)	0.0104 (4)	0.0145 (7)	0.0119 (6)	0.0026 (5)	0.0049 (4)	0.0010 (5)
Ô(Í)	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)
Ō(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)
Q(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)
$\tilde{O}(2)$	3262 (2)	503 (3)	2094 (3)	0.0083 (2)	0.0092 (4)	0.0217 (5)	0.0011 (3)	0.0072 (3)	0.0033 (4)
$\tilde{C}(\tilde{1})$	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)
$\tilde{C}(13)$	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)
$\hat{O}(W)$	1788 (3)	-2024(5)	-2600(4)	0.0108 (3)	0·040 (Ì)	0.0156 (5)	0.0026(5)	0.0032(3)	0.0033 (6)

Table 1. Atomic positional ($\times 10^4$) and anisotropic thermal parameters for L- α -GPE.H₂O

Table 1 (cont.)

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

x	У	Z
218(5)	422(8)	- 366 (6)
293 (5)	396 (8)	- 509 (7)
380 (6)	491 (9)	-342(7)
275 (5)	130 (8)	- 355 (7)
438 (5)	174 (8)	- 387 (6)
453 (5)	89 (8)	- 82 (6)
529 (5)	306 (8)	- 96 (6)
120 (5)	30 (9)	81 (7)
138 (5)	88 (8)	281 (6)
245 (5)	- 198 (7)	349 (7)
230 (6)	-410 (8)	130 (8)
30 (5)	-350 (9)	289 (6)
- 55 (5)	-200(8)	160 (7)
55 (5)	-152 (8)	524 (7)
172 (5)	-216(8)	-133 (7)
257 (6)	-198 (8)	-256 (6)
	x 218(5) 293(5) 380(6) 275(5) 438(5) 453(5) 529(5) 120(5) 138(5) 245(5) 230(6) 30(5) - 55(5) 55(5) 172(5) 257(6)	$\begin{array}{ccccc} x & y \\ 218(5) & 422(8) \\ 293(5) & 396(8) \\ 380(6) & 491(9) \\ 275(5) & 130(8) \\ 438(5) & 174(8) \\ 453(5) & 89(8) \\ 529(5) & 306(8) \\ 120(5) & 30(9) \\ 138(5) & 88(8) \\ 245(5) & -198(7) \\ 230(6) & -410(8) \\ 30(5) & -350(9) \\ -55(5) & -200(8) \\ 55(5) & -152(8) \\ 172(5) & -216(8) \\ 257(6) & -198(8) \end{array}$

(hkl and hkl) 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 hkl) was used in full-matrix least-squares refinement of the parameters listed in Table 1. The function minimized was $\sum [\Delta F/\sigma(F)]^2$ where $\sigma^2(F) = 0.1 +$ $0.001|F|^2$, and $\Delta F = |F_{meas}| - |F_{calc}|$. 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 $(\Delta f' = 0.2, \Delta f'' = 0.5)$ for phosphorus; $\Delta f' = 0.0$, $\Delta f'' = 0.1$ for oxygen). Independent refinements for enantiomeric crystal structures converged at R values of 0.029 and 0.039 respec-tively $(R = \sum_{\mathbf{h}} |\Delta F| / \sum |F_{\text{meas}}|)$, 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 $R_{anom} = \sum_{\mathbf{h}} |\Delta_{meas} - \Delta_{calc}| / \sum_{\mathbf{h}} |\Delta_{meas}|$ where $\Delta = (F_{\mathbf{h}}^2 - F_{\mathbf{h}}^2)$. 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. H₂O (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. H₂O.

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.H₂O

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.

N+ D L+ -8 1+ + 16 24 42 63 H+ D L+ -7 1+ 77 83	0 70 70 1 486 375 100 -154 2 285 280 -235 -300 3 346 342 451 487 4 37 57 2 49 5 229 227 234 497	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3 86 96 -14 -37 5 111 136 31 79 5 9 19 -37 2 6 12 77 6 12 77	1 109 100 129 75 2 113 113 14 -25 3 36 36 -3 13 4 48 68 -51 -82 5 28 28 16 6
2+ ++ ++ 3+ += ++ 4+ + 1 H= 0 (+ 1+ 111 114 2+ 11 114 2+ 11 114	6 0 0 -10 -01 0 0 0 0 0 -10 -01 0 22 22 1 10 0 251 268 1 236 220 -106 -126	H+ 2 L+ 5 0 47 65 1 131 152 72 204 2 70 74 1 33 3 86 89 146 146 4 114 119 2 80	7 76 80 H+ 4 (4 -3 0 217 225 1 183 184 -87 -139 2 78 93 -229 -161 3 61 63 -35 -14	0 127 128 -104 -97 1 157 158 -104 -97 2 79 36 -6 -25 5 147 155 -130 -54 5 50 51 -3 -4 5 115 116 -49 -72	H* 7 L* 2 0 44 47 1 154 154 48 44 2 75 77 -189 -12 3 96 97 -5 33 4 67 66 -18 -42 5 49 49 27 23
30 74 80 40 103 114 50 81 42 Me 0 Le -5	5 256 242 510 30: 6 241 226 -170 -377 5 201 148 -203 -326 5 172 170 -79 -167 7 106 103 43 -2	ne 2 Le 6 0 66 66 1 30 36 -61 -13 3 86 61 -14	5 100 105 26 72 6 62 63 109 111 7 26 26 3 -6	0 26 22 1 99 97 -17 5 2 29 23 2 7 3 42 40 47 41	He 7 Le 3 0 24 10 1 66 66 24 50 2 71 69 54 -33
2+ 10+ 109 1+ 77 8+ 4+ 8+ 72 5+ 8+ 71 6+ 51 5+	52 52 -41 -39 N= 3 Ce 1 0 453 513 1 371 370 274 480 2 48 79 202 134	2 61 82 -67 -56 6 69 50 -46 -51 He 2 Ce 7 0 124 122	0 48 71 1 142 139 -215 -209 2 103 104 33 -3 3 236 210 -94 -204 4 35 34 0 18 1 2 114 12 13	Ma 9 La 6 0 20 52 -1 9 6 0 1 Ma 6 La -3	* 39 *1 -19 -10 * 7 ** *1 0 ** *3 1 ** 21 **1 -20
H- 0 L+ -+ 1* 263 274 2* 137 139 3* 184 190 4* 173 181	5 63 66 -77 -61 6 177 166 636 289 7 91 92 -63 -26 6 89 87 -96 -83 7 80 80 -12 25	1 74 65 12 11 2 84 67 -51 66 3 35 29 7 -5 H- 7 L8 0 63 65	4 4 4 -13 -64 4 4 4 30 13 4 4 4 30 13	1 111 103 16 0	2 68 72 -2 4 H- & Lo -7 0 25 22 1 54 53 39 35
3+ 161 189 6+ 65 63 7+ 35 36 R+ 0 (+ -)	••• •••• •••• •••• •••• •••• •••• ••••• ••••• ••••••	1 29 24 12 1C 2 106 104 -10 -10 3 24 27 -24 -21 He 3 14 -7 0 42 47	1 215 214 -44 -330 2 156 128 140 253 3 159 159 73 88 4 21 20 -7 15 5 152 147 179 194 5 55 55 61 50	2 97 97 117 100 3 28 27 -7 -11 He 6 Le -6 0 76 73 1 203 200 133 110	H+ 8 L+ -6 0 120 115 1 96 95 66 75 2 123 119 27 34 3 23 22 13 -8
2* 115 115 3* 61 43 4* 121 125 5* 172 176 6* 4* 66 7* 67 90	3 138 142 -320 -321 4 46 44 3 1 5 204 208 -376 -308 6 41 40 2 -6 7 93 93 -81 -60 He 1 Le 3	1 52 53 52 71 2 79 61 28 0 1 47 66 7 7 6 29 52 -22 5 He 3 Le -6	7 49 48 52 39 He 4 Le 0 D 145 147 1 414 421 243 339 2 145 177 -330 -243 1 118 -44	2 50 50 -51 -23 3 101 99 36 -21 4 34 33 -7 -23 3 50 52 -24 -29 H* 6 L* -5	H+ 8 L+ -5 0 124 124 1 104 104 4 5 2 179 182 32 -2 3 42 40 0 2 4 49 49 0 13
H. 0 L2 1. 138 145 2. 226 226 3. 200 199 4. 211 214 5. 98 99	0 215 219 1 195 231 -121 -68 2 117 113 228 134 5 101 100 28 22 6 00 67 136 113 5 44 49 -37 -27	1 101 106 107 162 2 67 70 -20 -01 3 100 100 111 74 4 102 100 58 52 3 67 69 63 28 6 71 76 -22 -60	4 217 214 42 24 5 25 26 1 4 5 49 44 55 4 7 26 25 -3 7 14 4 14	1 172 175 -34 -54 2 103 103 -11 -10 3 147 151 55 85 • 34 57 -63 -37 5 49 54 9 49	H- 8 L+ 0 21 24 1 49 46 31 59 2 40 40 24 23 3 119 123 -143 -233 4 34 33 22 12
6+ 112 116 7+ 78 79 H= 0 L= -1 1+ 231 234	7 25 25 -1 -16 	7 41 43 3 -11 He 9 Le -5 0 212 200 1 172 174 24 31 2 115 111 -23 4 1 217 226 9 27	0 313 326 1 100 99 52 2 2 157 156 53 -60 3 67 62 150 123 6 82 82 26 8 3 106 101 -26 -75	0 9 8 1 151 156 162 99 2 32 35 -7 6 3 80 81 8 17 4 100 101 -168 -169	3 50 63 -56 -62 H 8 L3 0 86 88 1 110 115 -10 -8 2 100 115 162 171
3+ 196 193 4* 250 248 5+ 193 196 6* 21 20 7* 90 91	2 95 96 -71 -16 3 42 39 22 12 4 172 171 14 13 5 40 78 -61 4 6 65 46 7 5 7 60 61 -27 -51	a 43 45 5 -12 3 136 141 120 154 6 49 53 -20 -3 m- 3 La -4	6 82 86 -34 13 7 101 104 82 34 m. 4 L+ 2 0 81 87 1 184 173 10 -1	7 67 64 -23 -31 8 76 76 -73 -66 M* 6 (* -3) 0 58 60 1 16 16 16	3 44 41 -26 0 4 27 29 -22 -8 3 59 55 0 -21 H• 8 44 -2
H 0 L C 2 816 833 278 822 4 313 303 170 47 5 279 228 -217 -243 8 66 80	H 1 L 5 0 66 67 1 120 123 -07 -87 2 9 11 0 1 3 86 88 62 150 6 10 12 -39 -6	1 52 56	2 110 111 -156 -146 3 80 83 -9 -4 4 126 124 2 56 5 101 104 38 14 6 21 22 -18 6 7 57 59 -52 -47	2 40 40 -10 -48 3 124 124 -52 44 4 47 162 13 41 5 78 41 10 120 6 24 25 4 -1	1 169 174 -10 -49 2 82 81 -7 4 3 165 165 -86 -128 5 7 8C -24 -34 5 87 70 -87 -61
0 181 144 1 214 210 -773-1264 2 317 345 -401 -273 3 210 208 341 -273 4 25 250 46 110 5 185 185 -78 -45	5 02 02 -3 -15 6 43 44 -2 4 0 167 165 1 08 07 -1 2 2 17 176 -90 -4	H+ 3 L+ -3 0 46 47 1 222 226 -133 -254 2 145 144 -250 -192 3 392 395 -228 -248	H- 4 L+ 5 C 100 315 1 05 07 -77 -67 2 141 145 117 170 5 128 120 -20 4 4 68 48 -38 -17 5 8 48 -38 -17	C 51 56 1 85 87 -28 -18 2 192 189 6 -156 3 66 66 -19 -10 6 126 12C -164 -169 5 112 111 -42 -111	0 01 05 1 07 04 121 05 2 109 115 45 101 3 84 87 -31 -50 4 57 42 -36 15 5 28 28 22 14
27 24 10 7 01 03 52 32 8 0 0 -1 40 0 0 -2 0 590 712 1 102 150 03 148	\$ 107 137 -53 61 + 127 132 15 41 5 36 35 9 6 Me 1 Le 7 0 9 6 1 4 631 -30	115 115 -20 -11 115 115 -20 -11 0 7 67 37 38 1 67 68 0 0 1 15 115 -20 0 1 15 115 115 -20 -11 1 15 115 115 115 115 -20 -11 1 15 115 115 115 115 115 -20 -11 1 15 115 115 115 115 115 115 115 115 11	+ 114 12501 20 + 4 54 4 0 60 61 1 255 258 -164 -71 2 67 68 16 43	He 6 41 C 13" 141 1 141 14C 340 187 2 216 242 -161 -194 3 26 91 - 46	H- 8 L- 0 0 28 24 1 24 21 14 19 2 85 85 35 -14 3 9 14 0 -4 4 83 87 -8 18
2 228 227 -148 ++ 3 209 207 223 285 4 218 217 113 158 5 95 93 -45 -104 4 113 114 -47 -37 7 82 82 44 43	2 24 26 -3 -20 3 27 30 -19 -13 4 21 0 25 23 1 34 36 -20 -21	1 370 388 118 366 2 278 273 325 272 3 163 162 -189 -233 4 161 160 98 83 5 137 133 -96 -165 6 107 108 61 85 7 96 95 -116 -71	4 10 40 -7 0 5 100 103 -15 -4 He 4 10 5 0 165 162 1 00 57 23 2;	+ 227 223 0 47 5 40 46 33 44 4 80 80 36 36 46 H+ 6 L+ C 0 522 323 1 107 102 -8 -80	5 51 52 -35 -15 M- 8 L+ 3 C ICC 101 1 9 9 0 3 2 86 86 -7 -16 3 81 85 -87 -87
H- 0 L- 3 h 6+ 60 1 405 528 -051 8 2 10+ 10+ -368 -252 3 67 72 11 110 4 125 128 17 77	2 +3 +2 28 + H+ 2 L7 0 + 5 1 +0 +1 -+2 -2. 2 +0 +0 -13 -23	He 3 Le -1 0 253 265 1 225 235 67 -181 2 100 96 -96 -75 1 133 235 0 -4	2 06 06 -0 31 3 42 42 -24 14 4 102 102 -0 19 M- 6 40 50 1 115 116 -16 12	2 89 86 -57 -20 3 141 196 -50 4 4 17 71 403 -37 5 107 108 76 55 6 27 27 16 -1	A+ A3 A3 m+ B L+ 2 0 24 24 1 64 65 -10 6 2 80 82 -9 L
0 10 10	4 45 47 -40 -26 He 2 L4 -6 0 73 69 1 98 96 57 48	5 28 25 26 8 6 185 184 400 277 7 56 61 -13 -13 H+ 3 L+ 0	· · · · ·	0 110 111 1 86 82 -4 -43 2 172 133 -31 17 3 85 65 4 25 4 110 109 -75 -107	
1 261 268 -810 -345 2 134 138 -155 -8 3 190 190 -270 -17 4 136 181 -153 9 5 165 186 -180 -93	5 120 123	0 268 274 1 223 226 -152 -70' 2 25' 212 541 141 1 245 237 -137 -180 4 37 75 40 101 4 07 92 52 14	1 10 10 -7 0 10 10 -7 0 11 115 10 -3	5 41 42 -23 -19 6 104 106 -26 -24 H+ 6 44 2 7 151 153 1 14 77 -44 -72	no 9 Lo -6 0 26 26 3 90 91 32 32 2 16 16 -3 -6
7 1+ 35 -9 -7 H+ 0 L+ 3 0 1++ 138 1 1+ 32 -30 -17	0 40 38 1 74 75 -03 -39 2 132 117 31 8 3 130 142 5 32 4 26 25 26 13 5 137 158 35 152	6 156 158 25 -21 7 +5 +0 -6 -4 He 3 to 1 0 40 45	2 10 0 0 -1 3 93 93 40 33 4 44 46 0 1 He 1 La -6	2 40 71 -41 -21 3 190 2C3 -185 -124 4 92 9C 10 .25 5 80 91 0 4C	0 84 87 1 49 51 -5 24 7 75 74 -12 6 3 30 32 -13 -11
1 42 9C -41 11 4 96 10C 170 176 5 72 75 6 55 6 57 57 10 19	40 38 42 30 70 235 252 1 232 132 -28 -27 2 30 320 -355 -240	2 e13 62 76 61 3 46 30 -107 -100 4 73 75 -40 -70 5 76 94 -1 28 6 33 30 7 -2 7 5 40 -40 -40	1 228 229 32 -5 2 41 38 37 8 3 132 134 45 55 4 34 36 -35 -33 5 71 74 -63 -89	C 16 56 1 36 74 -5 15 3 117 161 -27 5 3 14 67 15 56 6 79 67 -66 11 5 11 67 -66 11	N= 0 (= 0 63 63 1 93 98 -27 -48 2 61 62 16 12 3 78 78 -12 6 - 51 10 10
1 209 111 -251 -112 2 85 86 -227 -118 3 75 79 -138 -22 4 109 112 -157 -50 5 80 80 -123 -32	3 102 108 -104 -02 4 2+5 2+2 -135 -205 5 38 00 -8 7 6 145 140 -5 -0 7 43 43 0 3	H* 5 (* 2 0 22 20 1 300 306 -23 52 2 103 106 -128 -167 3 38 36 -4 12	He 5 Le -5 0 36 54 1 80 82 -21 -65 2 171 100 110 87 3 54 57 -25 -26 6 81 84 36 37 5 40 41 91 -10	He 6 Le 6 0 114 130 1 43 45 25 14 2 108 111 2 -5 5 46 46 4 -27	- 72 74 -21 -10
He O Le 7 0 10 3 1 79 84 -101 15 2 41 43 -36 -3, 3 50 53 -21 37	0 280 108 1 55 52 -131 -155 2 55 56 -62 -68 3 155 161 -202 -177 6 71 57 -61 -23 5 91 91 62 62	4 20 10 -102 -72 5 105 110 20 37 6 131 134 -127 -21 7 50 64 -17 20 p+ 1 t+ 3	4 56 54 56 44 0 140 133 1 52 54 85 56	H- 4 L- 5 C Te 24 1 49 48 -27 -20 2 59 61 0 18	4 49 50 -4 -15 1 75 93 1 75 45 -4 -41 2 122 125 91 28
• 21 21 • 2 • 0 1• 8 0 9 3 1 19 16 • C 2 30 56 -136 -8E	* ** ** -0 -2; 7 77 76 -#1 -116 *** 2 L* -2 0 7 7	1 166 172 199 106 2 16 77 -17 -29 3 117 116 159 167 5 26 25 7 -1 2 -2 5 3 5 25 -17 -17	3 91 92 5 45 4 154 157 140 51 5 75 36 -10 -17 6 62 64 23 29	He 3 (2 - 7 C 2C 3 1 28 28 24 24 39 2 31 7C -15 2 3 4C 38 -25 -32	+ +3 +8 -5 15 + +6 (+ -1 0 31 36 1 320 124 75 20
He 1 (* -8 0 10 24 1 00 07 -30 -40 2 40 39 -21 -13 He 1 (* -7	2 201 200 -120 1 3 91 4- 127 80 4 210 -0190 5 124 127 -0 -51 6 175 174 42 11 7 45 42 -22 -22	He 3 Le 4 0 120 126 1 204 208 -106 -10 2 154 159 -163 -138 3 157 161 -120 -84	0 55 61 1 99 96 -220 -266 2 110 107 81 -44 3 46 43 0 2 4 98 99 -161 -65 5 40 34 -11 -34	He 3 Le -6 C 16: 177 1 3- 20 6 9 2 170 101 48 117 5 9 12 0 1 4 31 33 -62 -24	2 22 20 C 4 3 85 85 45 42 2 4 27 20 9 2 m- 9 L- 0 0 32 28 1- 37 38
0 46 45 1 21 18 35 6 2 22 21 19 21 5 30 51 -21 -20 4 51 49 42 10	H+ 2 L4 -1 7 136 132 1 144 144 -13 -24 2 121 121 223 214 3 178 347 -243 -406	+ 13C 133 -137 -36 5 119 121 -45 45 6 91 93 -36 -17 H- 3 4- 3 0 227 232	6 36 36 -13 -21 7 20 16 -16 -15 H- 5 L2 0 26+ 273 1 167 177 152 102	H4 7 L4 -5 0 10 0 1 40 51 01 07 2 62 61 1 -60 5 42 0792 -96	2 52 54 46 10 1 54 56 0 -21 4 44 49 8 25 m 9 6 - 3 0 28 22
He 1 Ce -6 0 12 75 1 275 184 -91 -1C2 2 100 111 22 13 3 140 187 0 -29 4 65 60 63 -5	4 156 150 571 106 5 106 103 41 101 4 95 98 -30 53 7 22 23 -22 -14 8 49 70 30 27 He 2 44 0	1 22 23 6 17 2 132 136 56 160 3 33 22 32 10 6 34 37 -11 -27 5 9 7 0 7	2 235 235 36 -35 3 146 146 98 14 4 239 238 16 -26 5 125 126 52 11 6 05 06 35 -5 7 52 52 27 35	+ 10 72 -3 -6 5 41 19 10 10 m 1 L -4 0 19 61 1 211 231 34 62 1 211 231 34 62	10 35 36 2 44 45 10 35 3 34 34 3 3 0 40 71
7 87 91 19 19 He 1 (4 -5 0 36 36 1 244 279 -129 52 2 199 156 -129 52	0 170 187 1 875 853 -629 897 2 510 202 -62 -66 3 251 243 76 -44 4 75 72 16 12	0 10 14 1 108 110 -25 0 2 56 56 0 12 3 06 106 -43 -13 6 7 47 0 12	H. 5 L1 0 161 159 1 6 0 -6 2 16 32 -9 -5 1 167 167 281 306	3 101 98 60 30 4 39 39 -57 -48 5 38 36 5 -9 H+ 1 L+ -3	2 52 55 13 35
8 67 68 19 52 6 177 176 145 544 8 176 116 -16 52 8 99 103 117 95	50 65 22 -2 7 76 77 -55 -63 8 51 67 26 -12 H- 2 6- 1	H- 5 L- 7 0 72 68 1 26 20 11 4	3 121 122 201 109 3 121 122 201 109 4 21 26 -5 -22 7 6 69 114 105	0 27 20 1 145 144 117 182 2 126 126 -6C -122 3 21 2C -36 -32 4 18 79 -95 -5C 2 3 35 -46 -49	me 10 ce -4 0 sl 50 1 35 35 0 -18 2 57 57_ 5 -12
No 217 221 1 97 26 21 5 2 27 27 378 -16 -77 3 17 6 0 4 172 180 -142 -87	0 130 126 1 336 539 -114 -247 2 68 67 1-6 111 1 271 172 122 -74 4 84 85 207 180	0 125 122 1 82 81 -11 5 2 131 126 -36 -56 He & Le -7	0 224 242 1 175 140 -30 -109 2 281 283 39 -119 3 105 104 64 63 4 172 170 21 46	48 51 -2 24 H 1 48 -2 0 25 18 1 213 219 140 101	#* 10 L * -3 0 #5 \$1 1 76 77 57 59 2 51 53 5 -6
3 55 59 -17 . Me 1 Le -3 0 137 187 1 256 270 -146 -104	+ 114 139 128 55 + 114 213 + 198 21 + 198 21	0 28 29 1 54 55 28 16 2 6 7 0 0 3 74 74 78 67 4 9 10 0 -4	6 20 32 10 31 7 66 68 27 27 0 236 262	- 131 127 67 -61 3 248 247 -10 -94 4 73 75 25 22 5 104 106 70 58 6 76 78 56 31	
2 252 260 -223 -257 3 107 104 11 184 4 127 123 -53 -58 5 208 200 41 53 6 10 16 0 5 7 64 69 29 41	1 224 232 -8 186 2 185 186 186 175 3 85 27 60 27 4 96 96 130 109 5 46 46 32 66 6 80 -82 -55 -56 7 60 61 -12 -57	H+ 4 (+ -6 0 500 501 1 79 82 +47 -54 2 220 221 163 108 3 67 84 -50 -60 4 105 109 -46 -58 5 63 62 0 -14	1 42 43 10 -16 2 124 131 -154 -124 3 112 124 -136 -124 4 145 144 -58 -4 5 43 41 -14 -45 6 68 71 -57 -12	He 1 (e -1) 0 (57) (70) 1 (47) (47) (4 (2)) 2 (24) (242) (350) (230) 3 (55) (50) (9 -3) 4 (57) (52) (3 -13) 5 (6 (6)) (21) (9)	H- 10 L - 1 0 87 77 1 41 44 26 10 2 86 89 67 66 H- 10 L 0 0 9 14
He 1	H= 2 L= 3 0 216 223 1 132 143 -153 -11 2 131 127 47 63 1 31 32 -42 1 4 45 47 -76 -62	H: 6 L: -5 0 41 34 1 81 87 -9 -71 2 146 153 -85 -32 3 139 139 -13 33 4 159 175 43 1-5	He 5 L 2 0 43 38 1 125 124 -187 -197 2 96 101 55 33 3 108 106 -16 -26 4 87 90 36 47 5 111 135 -119 -55	108 111 -8 5 10 28 29 107 107 104 54 2 87 85 -10 -75 3 210 234 -41 -44	1 0 16 -26 -15 2 35 36 -3 16 m-10 L- 1 0 9 13 1 8 11 0 1
0 211 251 -550 -554 7 52 54 -3 0 8 82 82 -51 -2-	7 113 1150 28 6 82 85 -271 7 57 61 14 17 84 2 L4 6 0 305 106	1 12 20 -10 -11 1 12 77 -12 -11 1 12 -14 1 10	6 93 98 20 32 H- 5 L- 3 0 354 354 1 70 75 -28 -24 2 85 88 25 76	5 50 50 23 C 5 78 50 60 100 6 33 13 13 -	

#123453 #1221456 #12294547 #1234567 #12234567

N - C(2)	1·495 (4) Å	N - C(2) - C(1)	112.2 (3)
C(2) - C(1)	1.483 (5)	C(2) - C(1) - O(1)	109.4 (3)
C(1) - O(1)	1.433 (4)	C(1)P	119.4 (3)
PO(1)	1.590 (2)	O(1)PO(2)	106.2 (1)
PO(2)	1.582 (2)	O(1)—P——O(3)	110.3 (1)
PO(3)	1.486 (2)	O(1) - P - O(4)	105.2 (2)
PO(4)	1.489 (3)	O(2)—P——O(3)	104·4 (1)
O(2) - C(11)	1.443 (4)	O(2) - P - O(4)	110.3 (1)
C(11)-C(12)	1.508 (4)	O(3)—P——O(4)	119.7 (1)
C(12)-O(12)	1.418 (4)	P O(2) - C(11)	122.3 (3)
C(12)-C(13)	1.517 (5)	O(2) - C(11) - C(12)	107.8 (2)
C(13)-O(13)	1.407 (4)	C(11)-C(12)-O(12)	107.9 (2)
		C(11)-C(12)-C(13)	111.0 (3)
$N \cdots O(1)$	2.827 (3)	O(12)-C(12)-C(13)	109.4 (3)
		C(12)-C(13)-O(13)	113.8 (3)
N-H C)·90–0·97 (5)		
О-Н ()•74–1•00 (6)		
C-H C	0.87-1.06 (5)		

Table 3. Bond distances and bond angles, with e.s.d.'s, for L- α -GPE.H₂O

bond lengths, 6.147 (9) Å, in GPE. H_2O is within the range 6.177 \pm 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 NH₃⁺ 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 NH₃⁺ 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 $[N \cdots O(13)$ distance 2.831 (4) Å]. Each hydroxyl group donates and accepts one hydrogen bond with $O \cdots O$ distances of $O(13)H \cdots O(W)$ 2.707 (4) Å, $O(12)H \cdots O(4)$ 2.693 (3) Å, $O(W)H \cdots O(12)$ 2.800 (4) Å and $O(W)H \cdots O(3)$ 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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