$\beta^2 = 24.4$ oe² when the protons are situated on F-F lines. Proton deviation from F-F directions (the magnitude of the intramolecular distance r(F-H) being preserved) lessen the theoretical values for β^2 so that with H-F-F angles exceeding 20° β^2 becomes less than the lower limit of its possible values. To summarize, it may be said that, according to the n.m.r. data, the protons in solid HF are situated at a distance of (0.95 ± 0.03) Å from the F atoms, involving a possible deviation from the F-F line not exceeding 10°.

It is also worthy of mention that according to the empirical formula of Pimentel & McClellan (1960), with F-F equal to 2.49 Å, the F-H bond length should approximately equal 1.02 Å, which is in agreement with our r(H-F) value in solid hydrogen fluoride.

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The crystal structure of POBr₃: space group and refinement by least squares.* By LIESELOTTE K. TEMPLETON and DAVID H. TEMPLETON, Lawrence Radiation Laboratory and Department of Chemistry, University of California, Berkeley, California 94720, U.S.A.

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Contrary to an earlier report, the X-ray diffraction data for POBr₃ are consistent with space group Pnma.

Olie & Mijlhoff (1969) (referred to below as OM) reported a crystal structure for phosphoryl bromide, POBr₃, which had been refined in space group $Pn2_1a$, but which deviated from *Pnma* by no more than 0.08 Å. OM stated that refinement in *Pnma* (with a block-diagonal least-squares program) 'proved to be disastrous' and that '*R* did not drop below 36%', whereas (with anisotropic thermal parameters) *R* was reduced to 11.3% in *Pn2*₁*a*. We found it incredible that one could not get approximately as good agreement in space group *Pnma* as in *Pn2*₁*a* with such slight deviations from the higher symmetry. Indeed, calculations we have made with the data of OM have reduced *R* below 11.3% in both space groups. We must conclude that there was some defect in the program used by OM or some error in using it.

Dr Olie kindly gave us a list of 432 non-zero structure factors. We refined the structure using the CDC-6600 computer and the full-matrix least-squares program of Dr Allan Zalkin of this laboratory. Scattering factors for neutral atoms were taken from Cromer & Waber (1965) with dispersion corrections for Br and P from Cromer (1965). OM used slightly different scattering factors and apparently neglected the dispersion corrections, but this difference certainly is not the origin of the divergence of our results. We assigned equal weights to the reflections for lack of knowledge of the experimental accuracies. The cell dimensions of OM were used: a=9.467(6), b=9.938(6),c=6.192(3) Å.

Starting with coordinates similar to those reported by OM (but naturally with Br(1) and Br(3) equivalent), four cycles of refinement in *Pnma* with individual isotropic thermal parameters reduced $R = \sum |\Delta F| / \sum |F_o|$ to 0.192 Further cycles yielded no significant improvement. With

individual anisotropic thermal parameters, eight cycles reduced R to 0.110 and $R_2 = \left[\sum (\Delta F)^2 / \sum F_0^2 \right]^{1/2}$ to 0.128. The final shifts in no case exceeded 10^{-3} times the respective estimated standard deviation. The resulting parameters are listed in Table 1 and the molecular dimensions are compared in Tables 2 and 3 with those found with the other space group. Observed and calculated structure factors (multiplied by 6) are listed in Table 4.

Table 1. Final parameters in space group Pnma

	Br(1)	Br(2)	Р	0
x	0.3469 (4)	0.4801 (6)	0.3102 (10)	0.174 (3)
y '	0.0790 (3)	4	$\frac{1}{4}$	4
Ζ	0.1799 (5)	0.6096 (8)	0.3799 (14)	0 ∙494 (4)
B_{11}^{*}	7.1 (2)	5.0 (3)	2.5 (4)	4 (1)
B_{22}	2. 6 (1)	5.8 (2)	$2 \cdot 2 (3)$	6 (2)
B ₃₃	4·2 (1)	3.3 (2)	2.4 (3)	3 (1)
B_{12}	−0 ·5 (1)	0	0	0
B_{13}	0.8 (2)	-1·6 (2)	0.5 (4)	2 (1)
B_{23}	-1·2 (1)	0	0	0

* The temperature factor is exp $\left(-\sum_{i}\sum_{j}h_{i}h_{j}b_{i}b_{j}B_{ij}/4\right)$.

Table 2. Bond distances

	Pnma	$Pn2_1a$		
P-Br(1) P-Br(2) P-Br(3) P-O OBr*	This work 2·131 (6) Å 2·147 (10) (2·131) 1·470 (29) 3·065 (27)	This work 2·118 (21) Å 2·148 (11) 2·147 (17) 1·445 (32) 3·092 (29)	OM 2·131 (11) Å 2·140 (6) 2·150 (11) 1·442 (18) 3·08 (2)	
0B	3.063 (27)	3.092 (29)	3.08 (2)	

* Atom in adjacent molecule.

^{*} Work done under the auspices of the U.S. Atomic Energy Commission.

Table 3. Bond angles

	Pnma	$Pn2_1a$		
	This work	This work	ОМ	
Br(1)-P-Br(2)	105·3 (3)°	106·2 (6)°	106·3 (4)°	
Br(1)-P-Br(3)	105.8 (2)	105.7 (8)	105.1 (3)	
Br(2)-P-Br(3)	(105.3)	103·5 (7)	105.3 (4)	
Br(1)-P-O	115.0 (6)	118.3 (28)	115.4 (17)	
Br(2)-P-O	109.8 (12)	109·6 (14)	109·5 (8)	
Br(3)-P-O	(115.0)	112.3 (25)	114.6 (18)	

Table 4. O	bserved and	d calcu	lated	structure	factors ((×6)
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FCA(0,0,0) = 3012

H-1 6 ()- ()		6 167 62	7 411 366	3 413 381	3 136 105	0 41 53
	0 301 137	3 482 501	1 240 207	4 14/ 189	4 45 42	1 253 223
2 4 38 389	1 748 271	4 66 34	4 276 200	5 79 77	E 273 272	2 172 141
4 431 387	2 352 552	5 360 366	6 411 443	A 12C 114	8 148 131	3 545 308
9 128 77	3 675 731	6 191 156	8 231 241	7 145 142	H.2# 5, 5	4 117 104
10 137 49	4 506 401	7 85 77	4 97 70	8 171 160	C 253 245	5 147 154
12 284 181	5 212 251	8 105 60	15 89 105	9 109 112	2 216 240	6 76 60
Hala Ca I	6 186 169	9 215 224	11 49 50	H,L: 4, 4	1 252 242	7 102 96
1 401 569	42 44	11 161 191	Mala 3. 4	0 213 211	4 203 196	8 81 50
2 402 438	8 280 254	12 31 41	0 166 153	1 104 89	5 97 85	9 130 120
0 111 142	4 147 152	11L3 2+ 3	1 354 381	2 241 225	6 148 144	H.L. 7. 2
7 461 448	10 121 106	J 267 199	2 94 75	3 85 53	6 86 101	C 232 192
11 243 249	11 104 101	1 523 483	3 358 352	4 231 231	H,L* 5, 6	1 297 306
		2 104 107	5 520 148	> 63 50	C 157 199	5 246 219
	0 517 568	3 401 456	0 45 100	6 47 41	4 82 77	6 105 94
4 104 372	2 205 264	5 303 211	/ 144 154	7 107 106	6 86 119	1 144 147
6 100 145	6 169 163	1 3/4 333	8 57 61	10 74 45	H.L. 6. C	+,L* 8, 0
9 150 344	6 141 104	1 240 252	A 144 141		5 165 372	1 755 249
12 105 120	4 354 390	0 103 101	"", L=	0 313 351	1 228 212	3 125 129
HULL C. J	8 107 101	11 45 50	1 217 233	1 02 74	2 15/ 143	5 161 201
1 2/2 350	0 101 100	11 45 50	1 217 87	2 61 70	3 442 520	7 87 106
5 105 112	1 1 7 7 1 40		2 232 234	3 115 110	4 147 137	8 // /5
9 49 51		0 1/0 103	4 123 134	0 21 203		4 9.7 68
11 100 95	0 440 544	1 144 312	- 135 81	8 70 33	6 431 528	H.L. 8. 1
H-1 3 (- 6	1 218 /16	1 97 121	0 141 165	0 314 330	7 140 142	0 117 102
0 569 572	2 107 149	5 97 121	8 101 199	10 210 224	\$ 200 207	1 153 112
2 605 391	3 179 2:0	5 141 167	···· · · · · · · · · · · · · · · · · ·	5 ICI 154	",L° 6, 1	2 255 234
4 298 2/1	5 199 188	5 58 40	1 262 262	N 1 N 1 N 1 N	1 151 297	1 157 152
6 354 367	5 267 251	1 261 225	2 143 148	2 123 146	1 103 124	· · · · · · · · · · · · · · · · · · ·
8 237 211	6 292 125	10 48 43	3 1 10 45	1 1 7 6 1 7 6	3 347 404	5 136 80
1.L. C. 5	1 97 80	1.1. 2. 5	6 92 10 1	6 P/ 117	5 165 152	7 87 84
1 117 135	9 76 67	0 259 238	5 174 243	H.17 5. 1	6 101 103	8 168 126
3 284 272	H.L. 1, 6	1 183 180	1 70 81	C 299 284	/ 88 76	9 65 64
5 69 85	0 133 170	2 1 08 93	H+L* 4+ C	1 238 202	P 138 105	H,L= R, 2
1 142 146	1 75 81	6 138 121	0 321 283	2 343 331	5 184 165	1 72 66
9 145 134	3 163 185	5 140 122	1 174 174	3 233 265	11 67 91	3 104 126
".L= C, C	4 69 51	6 195 188	3 550 608	4 284 288	H.L= 6, 2	5 84 74
3 103 184	0 117 124	/ 128 112	4 473 509	5 182 152	C 115 123	4.65 9. 1
4 200 200	1 02 74	"+L= 2+ 6	5 239 212	6 172 160	1 71 64	0 195 114
4 200 200		0 181 212	6 249 227	7 129 93	2 269 252	1 54 46
0 111 114	PAL 2 1.2 /		/ 161 16/			
8 110 120	1 60 61				2 1 21 1 22	6 1 67
8 110 120	3 50 54	3 240 252	8 345 362	9 143 114	4 171 167	4,L= 4, 2
8 110 120 H+L= C, 7	3 50 57 4 71 33 5 65 85	3 240 252	H 345 362 9 229 199	9 143 114 10 114 103	4 171 167 5 99 53	0 264 273
8 110 120 H+L= C, 7 1 138 169 3 122 124	3 50 59 4 71 33 5 65 85 Bala 2, 0	3 24C 252 5 75 68 6 115 130 7 56 43	H 345 362 9 229 194 10 H3 101	9 143 114 10 114 103 11 56 48	2 131 133 4 171 167 5 99 93 6 93 93	6 11 67 11,L= 1, 2 0 264 273 2 156 150 6 130 138
8 110 120 H+L= C, 7 L 138 169 3 122 124 5 109 137	3 50 57 4 71 33 5 65 85 H,L= 2, 0 C 161 113	3 24C 252 3 75 68 6 115 130 7 56 63 H.L. 2, 7	H 346 362 9 229 199 10 H3 101 11 125 140	9 143 114 10 114 103 11 56 48 H ₂ L= 5, 2	2 131 137 4 171 167 5 99 93 6 93 93 8 161 134 3 69 62	6 51 65 H,L= 9, 2 0 264 273 2 156 150 4 130 138 6 148 125
8 110 120 H.L. C. 7 1 138 169 3 122 124 5 109 137 H.L. 1	3 50 54 4 71 33 5 65 85 H.L. 2, 0 C 161 113 2 493 561	3 24C 252 3 75 68 6 115 130 7 56 63 H.L. 2, 7 0 122 150	H 345 362 9 229 194 10 H3 101 11 125 140 12 70 103 H,12 4, 1	9 143 114 10 114 103 11 50 48 H,L= 5, 2 0 253 182 1 214 152	2 (31 137 4 171 167 5 99 93 8 161 134 1 69 67 Pale 6	6 51 67 H,L= 4, 2 0 264 273 2 156 150 4 130 138 6 148 175 5 148 10, 0
8 110 120 H+L= C, 7 1 138 167 3 122 124 5 107 137 H+L= 1, 1 0 356 227	3 50 54 4 71 33 5 65 85 H,L= 2, 0 C 161 113 2 463 561 4 431 4,3	3 24C 252 3 75 68 6 115 130 7 56 63 H.L* 2, 7 C 122 15C 1 1C4 130	H 346 362 9 229 194 10 H3 101 11 125 140 12 70 103 H,L* 4, 1 5 793 826	0 143 114 10 114 103 11 50 48 H,L= 5, 2 0 253 182 1 214 152 2 450 486	5 131 137 4 171 167 5 99 63 6 93 93 8 161 134 7 69 67 1 128 121	6 51 65 11,L= 1, 2 0 264 273 2 156 150 4 135 138 6 148 175 ⊢,L= 10, 0 2 176 151
8 110 120 H.L. C. 7 1 138 167 3 122 124 5 107 137 H.L. 1, 1 0 356 227 1 209 168	3 50 5+ 4 71 33 5 65 85 H+L# 2, 0 C 161 113 2 463 561 4 431 453 5 651 648	3 24C 252 3 75 68 6 115 130 7 56 63 H.L. 2, 7 C 122 15C 1 1C4 130 2 123 1C4	H 346 362 9 229 194 10 H3 101 11 125 140 12 70 103 H,L,5 4, 1 5 703 826 1 487 534	9 143 114 10 114 103 11 50 48 H ₂ L# 5, 2 0 253 182 1 214 152 2 450 486 4 364 374	2 131 137 4 171 167 5 99 93 6 93 93 8 161 134 9 69 62 P.L. 6, 3 1 178 121 2 100 95	6 31 65 11,L= 3, 2 0 264 273 2 156 150 4 135 138 6 148 175 ⊢,L= 10, 0 2 17G 151 3 76 75
8 110 120 H.L= C. 7 1 138 167 3 122 124 5 107 137 H.L= 1, 1 0 356 227 1 289 168 2 699 677	3 50 5+ 4 71 33 5 65 35 H,LF 2, 0 C 161 1L3 2 463 561 4 431 4,3 5 601 648 6 179 132	i 24C 252 5 75 68 6 115 130 7 56 63 H.L. 2, 7 C 122 150 1 104 130 2 123 104 3 227 702	H 346 362 9 229 194 10 H3 101 11 125 140 12 7C 103 H,L, 4, 1 5 703 820 1 487 534 3 331 327	4 143 114 16 114 103 11 50 48 H,L5 5, 2 0 253 182 1 214 152 2 450 486 4 364 379 5 66 59	2 131 137 4 171 167 5 93 93 8 93 93 8 161 134 3 69 62 F.L. 6, 3 1 128 121 2 100 95 5 113 165	6 11 67 H,L= 4, 2 0 264 273 2 156 150 4 130 138 6 148 175 H,L= 10, 0 2 17G 151 3 76 7; 4 107 117
8 110 120 H.L.⇒ C. 7 L 138 167 3 122 124 5 109 137 H.L.≈ L. 1 0 356 227 1 289 168 2 699 677 3 700 758	3 50 57 4 71 33 5 65 85 H.L. 2, 0 C 161 113 2 403 561 4 431 471 5 601 6498 6 179 132 7 333 327	3 24C 252 5 75 68 6 115 110 7 56 63 H.L. 2, 7 C 122 15C 1 1C4 130 2 123 1C4 3 227 2C2 4 69 83	H 344 362 9 229 194 10 H3 101 11 125 140 12 7C 103 H,L5 4, 1 5 703 826 1 467 534 3 331 327 5 436 443	4 143 114 10 114 103 11 50 48 H+L= 5, 2 0 253 182 1 214 152 2 450 486 4 364 379 5 66 59 6 176 160	2 131 137 4 171 167 5 93 93 6 93 93 8 161 134 3 69 67 P.L. 6, 3 1 128 121 2 100 95 5 113 105 P.L. 6, 4	$\begin{array}{c} 6 & 51 & 67\\ (*, l = -9, 2\\ 0 & 264 & 273\\ 2 & 156 & 150\\ 4 & 137 & 138\\ 6 & 148 & 175\\ +, l = 10, & 0\\ 2 & 176 & 151\\ 3 & 76 & 77\\ 4 & 107 & 117\\ +, l = 10, l \end{array}$
8 110 120 H.L.= C. 7 1 138 167 3 122 124 5 107 137 H.L.= 1, 1 0 356 227 1 289 168 2 699 677 3 700 758 4 451 503	3 50 57 4 71 33 5 65 85 H+L# 2, 0 C 161 113 2 463 561 4 431 4,1 5 601 698 6 179 132 7 233 327 8 204 179	1 24C 252 5 75 68 6 115 130 7 56 63 H.L. 2, 7 0 122 15C 1 [C4 130 2 123 1C4 3 227 2C2 4 69 83 5 60 80	H 346 362 9 229 194 10 H3 101 11 125 140 12 7C 103 H,L> 4, 1 5 703 826 1 467 534 3 331 327 5 436 443 6 491 497	4 143 114 10 114 103 11 50 48 H→L= 5, 2 0 253 182 1 214 152 2 450 486 4 324 374 5 66 59 6 176 160 7 60 46	2 131 157 4 171 167 5 99 93 6 93 93 8 161 134 1 69 62 F.La 6, 3 1 178 171 2 100 95 5 113 105 F.La 6, 4 C 271 230	$\begin{array}{c} 6 & 71 & 67\\ 14, 12 & 47, 2\\ 0, 264 & 273\\ 2 & 156 & 150\\ 4 & 137 & 138\\ 6 & 148 & 175\\ 14, 12 & 10, 0\\ 2 & 17G & 151\\ 3 & 76 & 77, \\4 & 107 & 117\\ 14, 12 & 10, 1\\ 0 & 196 & 107\\ \end{array}$
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$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	1 2 C 2 2 2 3 7 5 68 6 115 130 7 56 63 H.L 2, 7 1 22 150 1 (24 130 2 123 104 3 227 2 2 3 24 6 121 2 166 121 4 70 56 12 75 86 H.L 3, 9 2 166 124 4 70 56 12 75 86 H.L 3, 9 2 16 128 4 70 56 12 75 86 H.L 3, 9 2 16 128 12 75 86 12 75 86	$\begin{array}{c} \text{H} & \text{J} & \text{J} & \text{J} & \text{J} & \text{J} & \text{J} \\ \text{g} & \text{g} & \text{g} & \text{g} & \text{g} \\ \text{g} & \text{g} & \text{g} & \text{g} \\ \text{l} & \text{g} & \text{g} & \text{g} \\ \text{g} \text{g} & \text{g} & \text{g} & \text{g} & \text{g} \\ \text{g} & \text{g} & \text{g} & \text{g} & \text{g} \\ \text{g} & \text{g} & \text{g} & \text{g} & \text{g} \\ \text{g} & $	$\begin{array}{c} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 &$	2 13 137 3 13 137 5 99 91 1 131 134 9 69 67 1 138 121 2 100 95 5 113 135 5 113 135 6 271 235 2 131 135 6 170 135 3 147 187 6 3 127 1 63 125 1 7 17 7 6 66 82 H _L	$\begin{array}{c} b & 1 \\ b & 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 2 \\ 1 \\ 1 \\ 1 \\ 1 \\$
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$ \begin{array}{c} 101 & 120\\ 114 = 6, 7\\ 1, 138 & 160, 7\\ 3, 122 & 124\\ 5, 150, 138 & 160, 7\\ 1, 122 & 124\\ 5, 150, 144 = 1, 1\\ 1, 240, 160, 240, 240, 240, 240, 240, 240, 240, 24$	3 50 5. 4 71 33 5 65 65 65 6 161 113 2 63 561 4 411 4. 4 41 4. 4 501 648 6 179 132 7 333 3. 8 230 3. 8 230 3. 8 230 3. 12 77 67 12 502 2. 14 250 2. 15 2. 15 2. 16 2. 17 1. 15 5. 16 2. 17 1. 18 2. 18 2. 19 1. 19 1. 19 1. 19 1. 19 1. 19 1. 19 1. 19 1. 19 1. 19 1. 10 5. 10 5.	1 2 C C 2 2 2 3 7 5 68 6 115 170 7 56 63 H.L C 2, 7 1 122 150 1 124 150 1 124 150 2 123 104 3 227 202 3 217 202 3 218 00 1 2 186 121 4 77 166 10 75 36 H.L 3, 12 3 26 20 1 2 186 121 1 2 186 128 1 2 186 186 186 186 186 186 186 186 186 186	H 154 162 9 220 194 10 H 101 11 125 140 12 77 103 1 407 524 1 120 120 1 211 120	$\begin{array}{c} \mathbf{n} & 1 + 1 + 1 + 1 \\ 1 + 1 + 1 + 1 \\ 1 + 1 + 5 + 5 \\ 1 + 1 + 5 + 5 \\ 2 - 2 + 5 + 2 \\ 2 + 1 + 1 + 5 \\ 2 + 2 + 5 + 1 \\ 2 + 1 + 1 + 5 \\ 2 + 2 + 1 + 1 \\ 5 + 5 + 1 \\ 5 + 1 + 1 \\ 5 + 1 \\ $	2 13 137 3 13 137 5 99 91 1 134 9 69 65 1 134 1 28 121 2 100 95 5 113 165 6 271 236 C 271 236 C 271 236 C 271 236 5 113 165 C 271 236 5 113 165 C 271 236 5 113 165 C 259 246 2 157 178 5 117 175 7 6 68 125 H ₁ = 66 85 C 56 66 65 1 116 86	$\begin{array}{c} \mathbf{u}_{1} = 1 & \mathbf{u}_{1} < \mathbf{z}_{1} \\ \mathbf{u}_{1} < \mathbf{z}_{1} < \mathbf{z}_{2} < \mathbf{z}_{1} \\ \mathbf{z}_{1} < \mathbf{z}_{2} < \mathbf{z}_{1} < \mathbf{z}_{1} < \mathbf{z}_{1} \\ \mathbf{z}_{1} < \mathbf{z}_{2} < \mathbf{z}_{1} < \mathbf{z}_{1} \\ \mathbf{z}_{1} < \mathbf{z}_{1} \\ \mathbf{z}_{1} < \mathbf{z}_{1} \\ \mathbf{z}_{1} < \mathbf{z}_{1} \\ \mathbf{z}_{1} \\ \mathbf{z}_{1} < \mathbf{z}_{1} \\ \mathbf{z}_{2} \\ $
$ \begin{array}{c} (151 \\ ($	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 1 \\ 2 \\ 2 \\ 2 \\ 3 \\ 7 \\ 5 \\ 6 \\ 6 \\ 115 \\ 170 \\ 6 \\ 6 \\ 115 \\ 170 \\ 175 \\ 6 \\ 6 \\ 175 \\ 6 \\ 175 \\ 100 \\ 121 \\ 120 \\ 121 \\ 120 \\ 120 \\ 120 \\ 120 \\ 120 \\ 100$	H 344 162 H 224 194 10 H 3101 11 125 140 12 7C 103 5 773 826 5 773 826 6 401 497 7 103 172 4 211 178 11 14C 159 4 213 178 12 51 201 2 04 162 3 753 207 4 513 201 2 198 165 5 7 43 1 251 201 2 198 165 5 7 43 1 251 201 2 198 165 1 251 201 2 198 165 3 753 207 4 514 11 1 10 10 10 1 2 10 10 1 2 10 10 1 2 10 10 1 2 10	$\begin{array}{c} \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $	2 1/1 1 17 1 1/1 17 5 93 91 1 1/2 1 17 6 93 91 1 1/2 1/2 1 1 1/2 1/2 1/2 1 2 1/2 1/2 1/2 1 2 1/2 1/2 1/2 1 2 1/2 1/2 1/2 1/2 1 2 1/2 1/2 1/2 1/2 1 2 1/2 1/2 1/2 1/2 1/2 1/2 1/2 1/2 1/2 1/	$\begin{array}{c} \mathbf{s}_{11} = 1\\ \mathbf{s}_{11} = 1\\$
L1 101 12 L1 101 12	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 1 \\ 2 \\ 2 \\ 2 \\ 3 \\ 7 \\ 5 \\ 6 \\ 6 \\ 1 \\ 15 \\ 16 \\ 15 \\ 16 \\ 16$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c} \begin{array}{c} & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 &$	2 101 107 2 101 107 3 101 107 4 101 107 4 101 107 5 0 07 1 100 100 5 100 1000 5	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$ \begin{array}{c} \text{m } 110 \ 123 \\ \text{m } 110 \ 123 \\ \text{m } 1 = 6 \ , 7 \\ 1 \ 125 \ 126 \\ 15 \ 126 \ 137 \\ \text{m } 1 \ 126 \ 126 \\ 126 \ 127 \ 124 \\ 10 \ 356 \ 227 \\ 1 \ 2497 \ 64 \ 214 \\ 2 \ 456 \ 526 \\ 4 \ 51 \ 526 \\ 5 \ 80 \ 536 \\ 8 \ 277 \ 243 \\ 9 \ 46 \ 273 \\ 1 \ 244 \ 214 \\ 1 \ 25 \ 556 \\ 1 \ 526 \ 4 \ 376 \ 410 \\ 5 \ 468 \ 431 \\ 1 \ 5 \ 468 \ 441 \\ 1 \ 5 \ 468 \ 441 \\ 1 \ 5 \ 468 \ 441 \\ 1 \ 5 \ 468 \ 441 \\ 1 \ 5 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 441 \\ 1 \ 448 \ 448 \ 441 \\ 1 \ 448 \ 448 \ 441 \\ 1 \ 448 $	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 1 \\ 2 \\ 2 \\ 2 \\ 3 \\ 7 \\ 5 \\ 6 \\ 6 \\ 115 \\ 170 \\ 150 \\ 6 \\ 175 \\ 6 \\ 6 \\ 115 \\ 170 \\ 175 \\ 6 \\ 175 \\ 100 \\ 121 \\ 121 \\ 100 \\ 1$	11 344 154 12 12 12 12 12 12 12 12 12 12 12 12 14 14 14 15 144 54 14 15 144 54 54 15 140 147 54 54 54 14 15 143 311 327 545 54	$\begin{array}{c} \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $	2 1/1 1 17 1 1/1 17 5 93 91 4 1/1 17 5 93 91 4 1/1 17 1 09 6 1 1/2 1	$\begin{array}{c} \mathbf{s}_{11} \\ \mathbf{s}_{11} \\ \mathbf{s}_{12} \\ \mathbf{s}_{11} \\ \mathbf{s}_{12} \\ \mathbf{s}_{11} \\ \mathbf{s}_{12} \\ \mathbf{s}_{11} \\ \mathbf{s}_{12} \\$
$ \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 $	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} 1 \\ 2 \\ 2 \\ 2 \\ 2 \\ 3 \\ 7 \\ 5 \\ 6 \\ 6 \\ 115 \\ 17 \\ 6 \\ 6 \\ 115 \\ 17 \\ 16 \\ 122 \\ 150 \\ 122 \\ 12$	1 3.54 16.2 1 1.25 1.40 1 1.25 1.40 1 1.25 1.40 1 1.25 1.40 1 1.25 1.40 1 4.37 3.1327 5 4.31 3.1327 6 4.31 1.43 1 4.31 3.1327 7 1.433 1.74 4 2.13 1.73 5 4.51 4.01 1 1.43 1.74 4 2.13 1.73 4 2.13 1.73 4 2.13 1.73 4 2.13 1.73 1 2.51 2.01 1.73 5 1.23 1.74 1.74 5 1.23 1.74 1.74 1 1.54 1.74 1.74 1 1.54 1.74 1.74 1 1	$ \begin{array}{c} \begin{array}{c} & 1 & 1 & 1 & 1 \\ (1 & 1 & 1 & 1 & 1 \\ (1 & 1 & 1 & 1 & 1 \\ (1 & 1 & 1 & 5 & 1 \\ (1 & 1 & 5 & 2 & 1 \\ (1 & 1 & 5 & 2 & 1 \\ (1 & 1 & 5 & 2 & 1 \\ (1 & 1 & 1 & 5 & 1 \\ (1 & 1 & 2 & 1 & 2 & 1 \\ (1 & 1 & 1 & 1 &$	2 101 107 2 101 107 3 101 107 6 93 91 114 1 69 65 1 108 107 1 108 100 1 108 100	$\begin{array}{c} \mathbf{u}_1 = \mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_1 \\ \mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_1 \\ \mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_1 \\ \mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_1 + \mathbf{v}_2 \\ \mathbf{v}_1 + \mathbf{v}_2 + \mathbf{v}_1 + \mathbf{v}_2 \\ \mathbf{v}_1 + \mathbf{v}_1 + \mathbf{v}_1 + \mathbf{v}_1 \\ \mathbf{v}_1 + \mathbf{v}_$

In space group $Pn2_1a$ one expects strong correlation between the parameters of Br(1) and Br(3), especially when these atoms are given independent anisotropic thermal parameters, and refinement difficulty would not be unexpected. However, refinement in this space group (with 45 independent parameters rather than the 28 used in *Pnma*) reduced *R* to 0·103 and R_2 to 0·119 without incident except considerably slower convergence than we achieved in *Pnma*. We started with the coordinates of OM and the thermal parameters listed in Table 1. The resulting coordinates correspond to bond distances and angles less symmetrical than those found in space group *Pnma*, and the thermal parameters correspond to more asymmetric motion. We regard these results to be unacceptable as a plausible model of the molecular structure, and we do not report the coordinates because we have no confidence in them.*

An examination of the discrepancies among the observed and calculated structure factors (for *Pnma*) revealed 11 that were larger than 15 electrons. Refinement in *Pnma* after removal of these 11 reflections resulted in R=0.097, $R_2=0.106$, and a bond distance P-O=1.49(2) Å. This sensitivity of the result to deletion of data suggests that more detailed analysis of this data set is unjustified without more specific knowledge of the accuracy of individual measurements, and that the standard deviations reported in this note are not to be taken too literally. The 11 reflections in question include the 10 which also gave the worst agreement in space group $Pn2_1a$, and therefore their poor agreement in *Pnma* cannot be taken as evidence for the non-centric group.

We conclude that there is no reason to reject *Pnma* as the correct space group, and that this description should be used unless and until some better evidence to the contrary is found.

Note added by Dr Olie, 3 May 1971: The refinement of our data by the Templetons shows that the conclusions drawn with respect to the molecular structure and intermolecular interactions are independent of the choice of $Pn2_1a$ or Pnma as the proper space group. Based on the information we have at present, we have no valid criterion for making a choice; therefore, the conclusion in the final lines of the Templetons' paper may be inverted to: 'We conclude that there is no reason to accept Pnma as the correct space group, and that this description should not be used unless and until some better evidence \cdots is found'.

In the case of POCl₃ (Olie, 1971), which has an analogous structure, we found, using photographic data weighting according to Cruickshank (1961) that the centric group could still be rejected on a 5% level.

* To anticipate a likely question, we report that the R test of Hamilton (1965), if applied to the R_2 ratio 0.128/0.119 = 1.08, gives the result that the centric group can be rejected at the 0.005 level. In our opinion the presence of systematic errors and incorrect weights makes this test inappropriate in the present case (cf. Ford & Rollett, 1970).

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