Table 34A-1-001. $PbHPO_4$. Fractional coordinates of atoms in phase I. The values of x and z of Pb and P atoms are fixed by symmetry in space group P2/c.

Atom		T = 293 K p = 1.50 GPa	T = 316 K p = 0 GPa
Pb	x	0.00	0.00
	y	0.2078(2)	0.19984(4)
	z	0.25	0.25
P	x	0.50	0.50
	y	0.7934(3)	0.79345(6)
	z	0.25	0.25
O(1)	x	0.3714(3)	0.37936(8)
	y	0.6558(3)	0.65892(5)
	z	0.4326(3)	0.43421(7)
O(2)	x	0.2565(2)	0.25625(6)
	y	0.9242(2)	0.92255(4)
	z	0.1245(2)	0.12780(5)
H	x	0.4837(16)	0.4839(7)
	y	0.4829(11)	0.5227(3)
	z	0.4852(16)	0.4811(5)
Ref.		[87Res]	[87Tun]

Table 34A-1-002. $PbHPO_4$. Interatomic distances and bond angles in phase I. $2R$: O–H–O distance, δ: H-site separation on the hydrogen bond, θ: angle P′–P–O(1) projected onto the (010) plane which characterizes the orientation of the PO_4 group around its two-fold axis.

	T = 293 K p =1.50 GPa	T = 316 K p = 0 GPa
Distance [Å]		
P–O(1)	1.551(2)	1.5497(4)
P–O(2)	1.528(2)	1.5287(4)
O(1)…O(3′) ($2R$)	2.441(3)	2.4701(7)
O(1)–H	1.193(7)	1.048(2)
H…H(δ)	0.310(17)	0.392(3)
Angle [°]		
O(1)–P–O(3)	109.09(16)	109.54(4)
O(2)–P–O(4)	111.98(17)	111.73(3)
O(1)–P–O(2)	108.73(7)	109.03(2)
O(1)–H–O(3′)	165.8(8)	174.8(3)
θ	27.97(8)	25.88(2)
Ref.	[87Res]	[87Tun]

Table 34A-1-003. $PbHPO_4$. Unit cell parameters at various T [83Hor].

T [K]	a [Å]	b [Å]	c [Å]	β [°]
158	4.6751(3)	6.6537(4)	5.7638(7)	97.04(2)
198	4.6776(3)	6.6524(4)	5.7687(7)	97.08(2)
228	4.6786(3)	6.6518(4)	5.7721(7)	97.09(2)
253	4.6801(3)	6.6504(4)	5.7744(7)	97.11(2)
273	4.6814(3)	6.6474(4)	5.7774(7)	97.14(2)
296	4.6829(3)	6.6447(4)	5.7798(7)	97.15(2)
310	4.6836(3)	6.6417(4)	5.7815(7)	97.15(2)
371	4.6868(3)	6.6474(4)	5.7891(7)	97.19(2)
421	4.6889(3)	6.6522(4)	5.7949(7)	97.21(2)

Table 34A-1-004. $PbHPO_4$. Unit cell parameters at various p [89Kat]. T = RT.

p	a [Å]	b [Å]	c [Å]	β [°]
0.10 MPa	4.6789(5)	6.6375(5)	5.7753(5)	97.135(8)
0.70 GPa	4.6605(8)	6.5827(14)	5.7466(14)	96.883(18)
0.85 GPa	4.6548(5)	6.5755(11)	5.7453(9)	96.870(11)
1.00 GPa	4.6492(6)	6.5636(10)	5.7392(9)	96.812(12)
1.12 GPa	4.6482(6)	6.5612(10)	5.7381(8)	96.806(11)
1.51 GPa	4.6363(4)	6.5357(11)	5.7275(8)	96.718(10)
2.00 GPa	4.6227(4)	6.5142(6)	5.7186(6)	96.616(8)
2.12 GPa	4.6225(4)	6.5022(18)	5.7137(6)	96.566(8)
2.30 GPa	4.6153(4)	6.4899(7)	5.7070(6)	96.529(8)
3.80 GPa	4.5717(6)	6.4213(12)	5.6715(7)	96.284(10)

Table 34A-1-005. $PbHPO_4$. $|d_{i\lambda}|$ at 223 K [88Kee]. $d_{i\lambda}$: susceptibility for second harmonic generation. λ = 1068.8 nm.

$\lvert d_{11}\rvert$	$\lvert d_{12}\rvert$	$\lvert d_{13}\rvert$	$\lvert d_{15}\rvert$	$\lvert d_{26}\rvert$	$\lvert d_{31}\rvert$	$\lvert d_{33}\rvert$	$\lvert d_{35}\rvert$
[$\cdot 10^{-12}$ mV^{-1}]							
0.90	0.14	0.42	0.38	0.15	0.44	0.50	0.49

Table 34A-1-006. $PbHPO_4$. Frequency [cm^{-1}] of A′ lattice modes obtained from Raman, infrared (IR) and hyper-Raman (HR). $X \parallel a$, $Y \parallel b$, $Z \parallel c^*$.

Raman				IR		HR	
T = 10 K				T = 4 K		T = 316 K	
$Z(XX)Y$	$X(YY)Z$	$X(ZZ)Y$		TO	A	TO	A
86.5	93.0	77.1	B_u(c)	79	B_u(c)	–	A_g
101.0	101.4	101.8	A_g	100	A_g	–	–
110.9	140.9	121.6	B_u(a)	112	B_u(a)	114	B_u(a)
146.1	149.4	146.8	?	–	–	–	–
155.5	–	–	B_u(a)	148	B_u(a)	142	B_u(a)
–	–	164.6	A_g	–	–	–	–
–	196.4	170.6	B_u(c)	168	B_u(c)	161	B_u(c)
176.7	178.2	177.6	A_g	187	A_g	–	–
248.6	256.8	228.7	2nd-order?	229	A_g	207	B_u(c)
[80Ohn]				[80Koc]		[90Shi]	

Table 34A-1-007. $PbHPO_4$. Frequency [cm^{-1}] of A″ lattice modes obtained from Raman, infrared (IR) and hyper-Raman (HR). $X \parallel a$, $Y \parallel b$, $Z \parallel c^*$.

Raman				IR		HR	
T = 10 K				T = 4 K		T = 316 K	
$Z(YX)Y$	$X(YX)Z$	$X(YX)Y$		TO	A	TO	A
52.2	52.1	52.0	B_g	–	–	–	–
81.0	81.1	81.0	B_g	–	–	–	–
100.7	100.0	99.9	B_g	–	–	–	–
146.5	–	146.7	?	–	–	–	–
–	147.8	–	A_u	146	A_u	141	A_u
159.1	158.8	159.0	B_g	–	–	–	–
174	173	–	B_g	–	–	–	–
189.8	182.5	207.7	A_u	182	A_u	177	A_u
201.6	201.3	200.8	B_g	–	–	–	–
308.0	292.2	308.5	2nd-order	–	–	–	–
[80Ohn]				[80Koc]		[90Shi]	

Table 34A-1-008. $PbHPO_4$. Eigenvalues and direction cosines of ^{207}Pb chemical shift tensors with respect to $x \parallel a, y \parallel b, z \parallel c^*$ [86Top].

	Eigenvalues $[\cdot 10^{-6}]$	Direction cosines		
		x	y	z
Phase I	$\sigma_1 = 2312$	0.9000	0.0000	−0.4350
$T = 42\,°C > \Theta_f$	$\sigma_2 = 164$	0.0000	1.0000	0.0000
	$\sigma_3 = 2494$	0.4350	0.0000	0.9000
Phase II	$\sigma_1 = 2312$	0.9036	±0.0044	−0.4284
$T = -25\,°C < \Theta_f$	$\sigma_2 = 130$	±0.0047	0.9928	±0.1195
	$\sigma_3 = 2526$	0.4258	∓0.1099	0.8969