Table 33A-1-001. KH_2PO_4 (KDP). Solubility *A* in water [62Kaf].

A [wt%]	*T* [°C]	*A* [wt%]	*T* [°C]	*A* [wt%]	*T* [°C]
12.88	0	20.04	25	29.00	50
14.00	5	21.90	30	33.40	60
15.50	10	23.65	35	37.05	70
16.87	15	25.10	40	41.30	80
18.45	20	26.90	45	45.50	90

Table 33A-1-002. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Metastable region for crystal growth in H_2O (KDP) and D_2O (DKDP) solutions [95Zai].

Saturation temperature [°C]	Temperature of first visible crystal [°C]
KDP	
44.5	–
54.0	7
54.0	8
61.3	20
61.3	16.5
71.4	33.2
71.4	34.7
75.1	43.1
75.1	41.8
DKDP	
56.4	7.0
71.6	18.0
76.5	34.0
77.7	26.5

Table 33A-1-003. KDP family. Unit cell parameters.

Crystals	a [Å]	c [Å]	c/a	T [°C]	Ref.
KH_2PO_4	7.4529(2)	6.9751(6)	0.9359(1)	25	67Coo
	7.452(2)	6.959	0.9338	20	47Ubb
KD_2PO_4	7.4697(3)	6.9766(5)	0.9340(1)	25	67Coo
	7.471_4	6.956_1	0.9310	20	47Ubb, 39Ubb *)
KH_2AsO_4	7.6295(6)	7.1605(8)	0.9385(2)	25	67Coo
	7.6300(4)	7.1630(3)	0.9388(2)	27, 25	65Des
	$7.625_6(10)$	$7.165_8(10)$	0.9396(2)	25	50Dic
KD_2AsO_4	7.6410(10)	7.1636(9)	0.9375(2)	25	67Coo
	7.641_5	7.165	0.9376	25	50Dic
RbH_2PO_4	7.608(8)	7.296(8)	0.9590(21)		64Hau
RbH_2AsO_4	7.7933(5)	7.4671(5)	0.9581(1)	25	67Coo
RbD_2AsO_4	7.8063(7)	7.4574(10)	0.9566(2)	25	67Coo
CsH_2AsO_4	7.9852(4)	7.8928(3)	0.9884(1)	25	67Coo
$NH_4H_2PO_4$	7.4991(4)	7.5493(12)	1.0067(2)	20	63Des
$ND_4D_2PO_4$	7.5193(9)	7.5400(19)	1.0028(4)	20	63Des, 42Ubb *)
$NH_4H_2AsO_4$	7.6944(4)	7.720(2)	1.0033(3)	25	67Che
	7.694(8)	7.718(8)	1.0031(21)		64Hau
	7.699(5)	7.729(5)	1.0039(13)		58Del

*) Recalculated in [67Coo].

Table 33A-1-004. KDP family. Unit cell parameters at Θ_f [67Coo].

Crystals	Θ_f or Θ_{IV-III} °C	Unit cell parameters [Å] at Θ_f or Θ_{IV-III}		c/a at Θ_f or Θ_{IV-III}	c/a at 25 °C
		a	c		
KH_2PO_4	−150	7.4256 (5)	6.9296 (9)	0.9332 (2)	0.9359 (1)
KD_2PO_4	− 51	7.4586 (7)	6.9559 (8)	0.9326 (2)	0.9340 (1)
KH_2AsO_4	−178	7.6034 (9)	7.1006 (11)	0.9339 (3)	0.9385 (2)
KD_2AsO_4	−112	7.6268 (14)	7.1195 (17)	0.9335 (4)	0.9375 (2)
	−114				
RbH_2AsO_4	−163	7.7727 (8)	7.4019 (10)	0.9523 (3)	0.9581 (1)
RbD_2AsO_4	−100	7.7950 (14)	7.4216 (19)	0.9521 (4)	0.9566 (2)
RbH_2PO_4	−126	7.586 (9)	7.250 (9)	0.9556 (23)	0.9590 (21)
CsH_2AsO_4	−130	7.9703 (14)	7.8329 (13)	0.9828 (4)	0.9884 (1)
$NH_4H_2PO_4$	−126	7.4710 (8)	7.5374 (18)	1.0089 (4)	1.0065 (2)
$NH_4H_2AsO_4$	− 57	7.6790 (12)	7.715 (2)	1.0047 (4)	1.0033 (3)

Table 33A-1-005. $KH_{2(1-x)}D_{2x}PO_4$. Unit cell parameters in the monoclinic phase (phase II).

	KDP 498 K in $P2_1$ or $P2_1/m$ cell	DKDP 403 K in $P2_1$ cell	DKDP ($x \approx 0.9$) RT in $P2_1$ cell	DKDP ($x \geq 0.98$) 77 K in $P2_1$ cell
a [Å]	7.47	7.471	7.45(1)	7.439(1)
b [Å]	14.49	14.711	14.71(2)	14.626(2)
c [Å]	7.33	7.167	7.14(1)	7.090(1)
β [deg]	92.2	92.34	92.31(1)	92.28(1)
Ref.	75Ito	74Tom	75Tho	76Ken

Table 33A-1-006. KD_2PO_4 (DKDP). Unit cell parameters in a face centered cell [74Nak].

T	293 K	232 K	211 K
a [Å]	10.557 (1)	10.549 (4)	10.602 (2)
b [Å]	10.557 (1)	10.549 (4)	10.498 (2)
c [Å]	6.975 (1)	6.961 (1)	6.961 (1)

Table 33A-1-007. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Unit cell dimensions and fractional coordinates at various temperatures [82Nel]. Neutron diffraction.

	KDP		DKDP	
	127(2) K	295(2) K	227(2) K	363(2) K
a [Å]	7.4264(10, 7)	7.4521(4, 4)	7.459(1, 1)	7.4794(10, 6)
c [Å]	6.931(3, 1)	6.974(2, 1)	6.957(2, 1)	6.995(2, 1)
x(H, D)	0.14867(7)	0.14757(12)	0.14901(8)	0.14736(11)
y(H, D)	0.22713(7)	0.22559(15)	0.22016(7)	0.22010(11)
z(H, D)	0.12266(22)	0.12161(47)	0.12098(14)	0.12113(22)
x(O)	0.14933(2)	0.14839(3)	0.14947(4)	0.14839(6)
y(O)	0.08283(2)	0.08264(3)	0.08091(4)	0.08108(6)
z(O)	0.12675(5)	0.12584(5)	0.12623(4)	0.12554(7)

Table 33A-1-008. KH_2PO_4 (KDP). Fractional coordinates of atoms in the paraelectric phase III. Neutron diffraction.

		RT [53Bac] (Small cell, $I\bar{4}2d$)	RT [53Bac] (Large cell, $F\bar{4}d2$)	132 K [55Bac] (Large cell, $F\bar{4}d2$)
K	x	0	0	0
	y	0	0	0
	z	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
P	x	0	0	0
	y	0	0	0
	z	0	0	0
O	x	0.1487(3)	0.0328(4)	0.0331(3)
	y	0.0828(3)	0.1158(40)	0.1161(3)
	z	0.1262(6)	0.1261(60)	0.1270(3)
H	x	0.1476(14)	0.961 0.937	0.960(2) 0.937(2)
	y	0.226(25) 0.274(25)	0.187 0.211	0.187(2) 0.210(2)
	z	0.125(3)	0.125	0.123(2) 0.127(2)

Table 33A-1-009. KH_2PO_4 (KDP). Fractional coordinates of atoms in the ferroelectric phase IV [55Bac]. Neutron diffraction.

		77 K (Orthorhombic cell, Fdd2)	
K	x	0	
	y	0	
	z	$\frac{1}{2}+0.016$ (2)	
P	x	0	
	y	0	
	z	0	
O		(OH)	(O)
	x	0.0339 (3)	0.1164 (3)
	y	0.1158 (3)	0.9661 (3)
	z	0.139 (2)	0.883 (2)
H	x	0.963 (1)	
	y	0.187 (1)	
	z	0.138 (4)	

Table 33A-1-010. KD_2PO_4 (DKDP). Fractional coordinates of atoms in phase III (T = 293, 232 K) and in phase IV (T = 212 K) [74Nak]. X-ray diffraction.

Atom		293 K	232 K	211 K	
P	x	0	0	0	
	y	0	0	0	
	z	0	0	0	
K	x	0	0	0	
	y	0	0	0	
	z	0.5	0.5	0.5178 (1)	
O	x	0.0338 (1)	0.0342 (1)	0.0343 (1)	0.1156 (1)
	y	0.1151 (1)	0.1152 (1)	0.1147 (1)	−0.0350 (1)
	z	0.1259 (2)	0.1265 (2)	0.1370 (3)	−0.1147 (3)

Table 33A-1-011. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Fractional coordinates and temperature parameters at 20 °C [73Nak]. U_{ij} is defined by Eq. (d) in Introduction. Small cell $I\bar{4}2d$. Values for KD_2PO_4 are in brackets. X-ray diffraction.

Atom	x	y	z	U_{11} [Å^2]	U_{22} [Å^2]	U_{33} [Å^2]	U_{12} [Å^2]	U_{23} [Å^2]	U_{31} [Å^2]
K	0	0	0.5	0.0213 (3)	0.0213 (3)	0.0141 (2)	0	0	0
	[0]	[0]	[0.5]	[0.0215 (2)]	[0.0215 (2)]	[0.0146 (1)]	[0]	[0]	[0]
P	0	0	0	0.0122 (3)	0.0122 (3)	0.0155 (2)	0	0	0
	[0]	[0]	[0]	[0.0123 (2)]	[0.0123 (2)]	[0.0172 (2)]	[0]	[0]	[0]
O	0.1486 (1)	0.0825 (1)	0.1262 (2)	0.0154 (3)	0.0157 (3)	0.0199 (3)	0.0020 (3)	−0.0042 (3)	−0.0066 (3)
	[0.1489 (1)]	[0.0813 (1)]	[0.1259 (2)]	[0.0152 (2)]	[0.0161 (2)]	[0.0201 (2)]	[0.0022 (2)]	[−0.0043 (2)]	[−0.0060 (2)]

Table 33A-1-012. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Anisotropic temperature parameters [82Nel]. U_{ij} is defined by Eq. (d) in Introduction. Neutron diffraction.

	KDP		DKDP	
	127 K	295 K	227 K	363 K
U_{11}(K)	0.00922(5) Å²	0.0204(2) Å²	0.0161(2) Å²	0.0259(4) Å²
U_{33}(K)	0.0066(1)	0.0141(2)	0.0103(3)	0.0163(6)
U_{11}(P)	0.0052(1)	0.0106(1)	0.0088(1)	0.0139(2)
U_{33}(P)	0.0081(1)	0.0138(2)	0.0141(2)	0.0174(5)
U_{11}(H, D)	0.0172(2)	0.0223(3)	0.0157(2)	0.0205(3)
U_{22}(H, D)	0.0166(4)	0.0249(7)	0.0163(3)	0.0238(6)
U_{33}(H, D)	0.0199(2)	0.0268(4)	0.0198(2)	0.0255(5)
U_{23}(H, D)	−0.0007(4)	−0.0020(9)	−0.0018(3)	−0.0033(5)
U_{31}(H, D)	−0.0018(3)	−0.0019(6)	−0.0015(3)	−0.0026(4)
U_{12}(H, D)	−0.0005(2)	−0.0005(3)	−0.0006(3)	−0.0005(3)
U_{11}(O)	0.0068(1)	0.0144(1)	0.0113(1)	0.0182(2)
U_{22}(O)	0.0070(1)	0.0142(1)	0.0116(1)	0.0184(2)
U_{33}(O)	0.0091(1)	0.0186(1)	0.0148(1)	0.0227(5)
U_{23}(O)	−0.0017(1)	−0.0039(1)	−0.0028(1)	−0.0049(2)
U_{31}(O)	−0.0050(1)	−0.0054(1)	−0.0041(1)	−0.0072(2)
U_{12}(O)	0.0006(1)	0.0019(1)	0.0015(1)	0.0025(2)

Table 33A-1-013. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Anisotropic temperature parameters [Å²] at various temperatures and pressures [82Tib]. (a)–(h) correspond to the conditions indicated in Table 33A-1-017 and Table 33A-1-018. U_{ij} is defined by Eq. (d) in Introduction. Neutron diffraction.

	U_{11}(K)	U_{11}(P)	U_{11}(O)	U_{22}(O)	U_{12}(O)	$U_{11} = U_{22} = U$(H, D)
KDP						
(a)	0.0213(8)	0.0126	0.0162(17)	0.0160(17)	0.0015(5)	0.0266(17)
(b)	0.0186(5)	0.0108	0.0138(9)	0.0151(9)	0.0022(3)	0.0241(11)
(c)	0.0194(15)	0.0121(10)	0.0148	0.0148(6)	0.0015	0.0255(29)
(d)	0.0175(7)	0.0106(4)	0.0153	0.0153(3)	0.0022	0.0254(14)
(e)	0.0062(2)	0.0036	0.0051(4)	0.0053(4)	0.0003(1)	0.0161(6)
DKDP						
(f)	0.0235(8)	0.0146(4)	0.0176(3)	0.0173(3)	0.0021(4)	0.0225(9)
(g)	0.0189(7)	0.0124(4)	0.0154(3)	0.0157(3)	0.0019(3)	0.0230(10)
(h)	0.0155(8)	0.0090	0.0110(15)	0.0116(15)	0.0004(5)	0.0136(14)

Table 33A-1-014. KH_2PO_4 (KDP), $KH_{2(1-x)}D_{2x}PO_4$ (x = 0.95). Fractional coordinates and temperature parameters [$\cdot 10^5$ Å^2] at 293 K [88Tun]. U_{ij} is defined by Eq. (d) in Introduction. Neutron diffraction.

Atom	Parameter	KDP	95% DKDP
P	U_{11}	1314(11)	1431(9)
	U_{33}	1635(16)	1835(16)
K	U_{11}	2248(22)	2376(18)
	U_{33}	1677(25)	1625(23)
O	x	0.14839(4)	0.14888(3)
	y	0.08263(4)	0.08111(3)
	z	0.12586(5)	0.12595(4)
	U_{11}	1666(10)	1744(7)
	U_{22}	1644(10)	1783(8)
	U_{33}	2110(10)	2171(8)
	U_{12}	185(9)	198(6)
	U_{13}	–544(10)	–575(8)
	U_{23}	–381(10)	–395(7)
H(D)	x	0.14762(15)	0.14821(7)
	y	0.22582(20)	0.22038(6)
	z	0.12098(63)	0.12087(12)
	U_{11}	2430(36)	2122(17)
	U_{22}	2817(91)	2412(25)
	U_{33}	2868(46)	2553(19)
	U_{12}	–95(37)	–45(12)
	U_{13}	–131(75)	–192(22)
	U_{23}	–253(110)	–295(26)

Table 33A-1-015. KH_2PO_4 (KDP). Interatomic distances [Å] at different temperatures [55Bac]. O and O_H are two sorts of hydrogen atoms at 77 K: O_H with the nearest hydrogen atom 1.04 Å away, O with the nearest hydrogen atom 1.44 Å away. The primed and unprimed atoms are in an opposite z direction relative to the central atom of the PO_4 tetrahedron. Neutron diffraction.

Bond	RT	132 K	77 K	
			obs	mean
P–O_H	1.538 (5)	1.538 (4)	1.583 (20)	1.545
P–O			1.508 (20)	
O_H–O_H	2.528 (7)	2.528 (9)	2.521 (6)	2.535
O–O			2.549 (6)	
O–O'_H	2.503 (8)	2.503 (5)	2.519 (20)	2.515
O_H–O′			2.512 (20)	
O–H–O	2.487 (5)	2.475 (4)	2.486 (4)	
O_H–H	1.07 (1)	1.07 (1)	1.050 (14)	
O–H	1.42 (1)	1.41 (1)	1.430 (14)	
K–O_H	2.888 (6)	2.870 (3)	2.896 (30)	2.864
K–O			2.833 (30)	
K–O'_H	2.819 (4)	2.802 (5)	2.812 (10)	2.795
K–O′			2.777 (10)	

Table 33A-1-016. KD_2PO_4 (DKDP). Bond lengths and angles related to PO_4 tetrahedron and O–D–O bonding [74Nak]. X-ray diffraction.

	293 K	232 K	211 K	
Angle between pairs of bonds related by symmetry axis along *c*	110°34′ (6)	110°28′ (9)	105°38′ (10)	116°05′ (12)
Lengths of P–O bond [Å]	1.541 (1)	1.544 (1)	1.578 (2)	1.509 (2)
Angle between O–D–O bonds and *x*–*y* plane	17′ (2)	28′ (3)	17′ (4)	
Length of O–D–O bond [Å]	2.519 (1)	2.521 (2)	2.530 (2)	

Table 33A-1-017. KH_2PO_4 (KDP). Structural parameters at various temperatures and pressures. The origin of the positional parameters (*X*, *Y*, *Z*) is on P atom [82Tib]. *d*: P–O distance. 2*R*: O–O distance. δ: distance between two H sites in the hydrogen bond. d_{xy}, δ_{xy}: projections of *d* and δ onto the *xy* plane. See Fig. 33A-1-018 for other symbols. Neutron diffraction.

	(a)	(b)	(c)	(d)	(e)
T [K]	295(2)	295(2)	295(2)	295(2)	71(2)
p [$\cdot 10^8$ Pa]	$\lesssim$0.050	14(1)	$\lesssim$0.050	16.5(5)	12(1)
Θ_f [K]	123	47	123	15	68(2)
a [Å]	7.453(1)	7.344(4)	7.453(1)	7.329(3)	7.317(4)
c [Å]			6.973(1)	6.856(3)	
H *X* [Å]	1.094(6)	1.112(4)	1.106	1.119	1.111(3)
Y [Å]	1.676(6)	1.660(5)	1.691(8)	1.676(6)	1.688(5)
Z [Å]			0.872(14)	0.839(8)	
O *X* [Å]	1.110(2)	1.116(2)	1.106(2)	1.119(1)	1.1130(6)
Y [Å]	0.621(2)	0.602(2)	0.614(2)	0.598(1)	0.6047(6)
Z [Å]			0.878(3)	0.868(2)	
d_{xy} [Å]	1.271(2)	1.268(2)	1.265(2)	1.269(2)	1.2667(7)
d [Å]			1.540(2)	1.537(2)	
r [Å]	1.055(7)	1.058(6)	1.077(9)	1.078(7)	1.084(5)
2*R* [Å]	2.484(4)	2.468(3)	2.498(5)	2.469(3)	2.449(3)
δ_{xy} [Å]	0.375(12)	0.351(9)	0.344(17)	0.313(11)	0.280(9)
δ [Å]			0.344(17)	0.315(11)	
θ [°]	60.77(5)°	61.65(4)°	60.95(5)°	61.89(5)°	61.49(2)°

Table 33A-1-018. KD_2PO_4 (DKDP). Structural parameters at various temperatures and pressures. The origin of the positional parameters (*X*, *Y*, *Z*) is on P atom [82Tib]. See Table 33A-1-017 and Fig. 33A-1-018 for the definitions of the parameters. Neutron diffraction.

	(f)	(g)	(h)
T [K]	295(2)	295(2)	193(2)
p [$\cdot 10^8$ Pa]	$\lesssim$0.050	16.5(8)	11(1)
Θ_f [K]	222	174	189(2)
a [Å]	7.469(1)	7.342(3)	7.357(4)
c [Å]	6.976(1)	6.864(3)	
D X [Å]	1.110(2)	1.126(2)	1.108(4)
Y [Å]	1.644(2)	1.643(2)	1.636(4)
Z [Å]	0.840(3)	0.838(5)	
O X [Å]	1.112(1)	1.1218(9)	1.117(2)
Y [Å]	0.603(1)	0.5881(8)	0.593(2)
Z [Å]	0.882(2)	0.875(1)	
d_{xy} [Å]	1.265(1)	1.267(1)	1.265(2)
d [Å]	1.542(1)	1.540(1)	
r [Å]	1.041(3)	1.055(2)	1.043(3)
$2R$ [Å]	2.529(3)	2.495(2)	2.493(4)
δ_{xy} [Å]	0.448(5)	0.385(4)	0.406(8)
δ [Å]	0.452(5)	0.387(4)	
θ [°]	61.55(6)°	62.33(4)°	62.03(9)°

Table 33A-1-019. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Structure parameters of H_2PO_4 ion [82Nel]. φ and ψ are the inclinations of O...O and H–H lines to the *XY* plane, respectively. See Table 33A-1-017 for the definitions of the other parameters. The primed parameters are the corrected values for librational or riding motion. p is the structure parameter of the first column. Neutron diffraction.

	KDP			DKDP		
	127 K	295 K	$\Delta p/\Delta T$ [$\cdot 10^{-4}$ Å K^{-1}] or [$\cdot 10^{-4}$ °K^{-1}]	227 K	363 K	$\Delta p/\Delta T$ [$\cdot 10^{-4}$ Å K^{-1}] or [$\cdot 10^{-4}$ °K^{-1}]
$2R$	2.4832(5) Å	2.4945(5) Å	0.68(4)	2.5226(6) Å	2.5268(8) Å	0.31(7)
$2R'$	2.4822(8)	2.4919(9)	0.58(7)	2.5211(12)	2.5237(17)	0.19(14)
r	1.0720(7)	1.0658(14)	−0.37(9)	1.0394(9)	1.0402(12)	0.06(11)
r'	1.0819(8)	1.0734(15)	−0.51(10)	1.0439(10)	1.0427(13)	−0.08(12)
δ	0.341(1)	0.367(2)	1.56(13)	0.449(1)	0.451(2)	0.14(14)
δ'	0.320(3)	0.347(3)	1.62(25)	0.437(2)	0.441(2)	0.30(21)
d	1.5427(2)	1.5403(4)	−0.14(2)	1.5423(5)	1.5397(7)	−0.19(6)
d'	1.5440(6)	1.5438(7)	−0.01(6)	1.5442(7)	1.5435(9)	−0.05(8)
θ	60.99(1)°	60.89(2)°	−6(1)	61.57(2)°	61.35(3)°	−16(3)
ψ	5.5(5)	7.4(10)	113(70)	7.2(3)	6.9(4)	−22(36)
φ	0.56(1)	0.27(2)	−17(1)	0.39(1)	0.17(2)	−16(1)
φ'	0.59(1)	0.36(2)	−14(1)	0.44(1)	0.27(2)	−10(1)

Table 33A-1-020. KH_2PO_4 (KDP), $KH_{2(1-x)}D_{2x}PO_4$ (x = 0.95). Lattice parameters [Å], interatomic distances [Å] and angles [°] at 293 K [88Tun]. Angles θ, φ, ψ and labeling of atoms, see Fig. 33A-1-018. For the K atoms, the distances and angles are given for both the nearest-neighbor (NN) and next-nearest-neighbor (NNN) O atoms. Superscript to atom symbol: (a) $-y$, $1/2 - x$, $1/4 + z$; (b) x, $1/2 - y$, $1/4 - z$; (c) $-x, -y, z$; (d) $y, x - 1/2, 1/4 + z$. Neutron diffraction.

	KDP	95 % DKDP
Lattice parameters [Å]		
a	7.4521(4)	7.4690(5)
c	6.974(2)	6.975(2)
Distances [Å]		
P–O	1.5403(4)	1.5412(3)
K–O[a] (NN)	2.8274(3)	2.8272(3)
K–O (NNN)	2.9000(8)	2.9001(7)
O–H(D) (r)	1.0677(16)	1.0408(5)
H(D)...O[b]	1.4276(15)	1.4829(5)
O...O[b] ($2R$)	2.4946(6)	2.5230(5)
H(D)...H(D)[b] (δ)	0.3647(28)	0.4462(9)
Angles [°]		
O–P–O[c]	110.52(3)	110.50(3)
θ	60.89(1)	61.42(1)
O[a]–K–O[d] (NN)	144.34(2)	144.36(2)
O–K–O[c] (NNN)	51.75(2)	51.78(2)
O–H(D)...O[b]	177.23(40)	177.15(8)
φ	0.265(19)	0.291(17)
ψ	8.8(1.4)	7.4(2)

Table 33A-1-021. KH_2PO_4 (KDP). Structural data under hydrostatic pressure at RT [89End]. Space group: $I\bar{4}2d$. P at (0, 0, 0), K at (0, 0, 1/2), O at (x_0, y_0, z_0). B is defined by Eq. (e) in Introduction. φ: inclination angle of the hydrogen bond to (001) plane. For θ see Fig. 33A-1-018. X-ray diffraction.

p [GPa]	0.0001	0.4	0.9	1.4	2.0	2.6	3.2	3.8	4.5	5.0	5.4
Lattice parameter											
a [Å]	7.4596(11)	7.425(2)	7.395(2)	7.351(2)	7.319(2)	7.278(2)	7.247(1)	7.225(4)	7.197(1)	7.174(5)	7.163(2)
c [Å]	6.9795(9)	6.957(2)	6.921(2)	6.886(2)	6.849(2)	6.807(3)	6.774(1)	6.747(3)	6.706(1)	6.681(5)	6.676(2)
Positional parameter											
x_O	0.1478(3)	0.1496(12)	0.1483(11)	0.1535(24)	0.1531(13)	0.1539(15)	0.1552(20)	0.1556(25)	0.1568(22)	0.1566(30)	0.1564(22)
y_O	0.0826(3)	0.0825(14)	0.0828(13)	0.0839(29)	0.0815(15)	0.0812(17)	0.0769(25)	0.0736(32)	0.0739(29)	0.0721(40)	0.0728(28)
z_O	0.1260(4)	0.1244(12)	0.1257(11)	0.1273(22)	0.1287(14)	0.1297(15)	0.1296(21)	0.1298(25)	0.1307(23)	0.1312(29)	0.1301(23)
Temperature parameter											
B_K	1.58(2)	1.8(2)	1.7(2)	1.6(4)	1.4(2)	1.4(3)	1.8(4)	1.1(4)	1.4(4)	1.4(5)	1.3(4)
B_P	1.14(2)	1.3(2)	1.4(2)	1.2(4)	1.3(2)	1.2(3)	1.6(4)	1.0(4)	1.0(4)	0.6(5)	1.1(4)
B_O	1.39(3)	1.8(3)	2.0(2)	1.8(6)	1.8(3)	1.7(3)	2.5(5)	1.7(6)	2.0(5)	1.7(8)	2.1(5)
R_{O-O} [Å]	2.498(4)	2.488(21)	2.473(19)	2.443(43)	2.467(22)	2.457(24)	2.509(36)	2.550(47)	2.536(42)	2.554(57)	2.539(41)
P–O [Å]	1.539(2)	1.535(91)	1.528(81)	1.556(18)	1.545(99)	1.544(11)	1.532(15)	1.521(18)	1.525(16)	1.516(22)	1.510(16)
O–O in PO_4 [Å]	2.526(4)	2.536(19)	2.512(17)	2.571(37)	2.539(20)	2.533(22)	2.511(31)	2.487(38)	2.495(33)	2.473(46)	2.472(34)
O–P–O [deg]	110.3(2)	111.4(7)	110.6(6)	111.4(12)	110.4(7)	110.3(8)	110.1(11)	109.7(13)	109.8(12)	109.3(16)	109.8(12)
θ [deg]	60.80	61.12	60.82	61.35	61.97	62.18	63.64	64.69	64.75	65.27	65.03
φ [deg]	0.3074	0.2051	0.2261	0.7397	1.174	1.479	1.417	1.446	1.725	1.859	1.525

Table 33A-1-022. KD_2PO_4 (DKDP). Structural data under hydrostatic pressure at RT [89End]. Deuteration rate: 99.7%. Symbols are the same as those of Table 33A-1-021. X-ray diffraction.

p [GPa]	0.0001	1.3	2.7	3.3	3.9	4.5	4.9	5.2	5.6	6.5
Lattice parameter										
a [Å]	7.4696(4)	7.375(5)	7.297(9)	7.264(3)	7.226(7)	7.201(6)	7.186(1)	7.199(3)	7.170(1)	7.155(2)
c [Å]	6.9750(4)	6.874(3)	6.974(2)	6.762(2)	6.713(5)	6.698(4)	6.680(1)	6.673(3)	6.667(1)	6.641(5)
Positional parameter										
x_O	0.1489(2)	0.1502(23)	0.1581(29)	0.1556(33)	0.1576(66)	0.1574(63)	0.1530(19)	0.1630(70)	0.1577(27)	0.1516(30)
y_O	0.0809(2)	0.0795(20)	0.0818(30)	0.0783(36)	0.0819(67)	0.0749(77)	0.0731(21)	0.0713(91)	0.0705(31)	0.0697(36)
z_O	0.1260(2)	0.1305(17)	0.1289(24)	0.1288(29)	0.1348(65)	0.1243(53)	0.1316(19)	0.1315(91)	0.1272(30)	0.1361(31)
Temperature parameter										
B_K	1.61(2)	1.1(2)	2.3(2)	1.8(2)	1.8(2)	1.2(3)	1.6(3)	1.7(3)	1.2(4)	0.8(4)
B_P	1.20(2)	1.8(2)	1.2(2)	2.4(3)	1.7(2)	2.4(4)	1.2(3)	1.5(4)	1.8(5)	2.5(5)
B_O	1.40(3)	2.5(2)	2.6(2)	2.6(3)	2.5(3)	2.6(3)	1.8(4)	2.3(6)	2.5(5)	1.0(5)
R_{O-O} [Å]	2.5263(30)	2.510(29)	2.449(47)	2.475(52)	2.433(70)	2.540(70)	2.554(30)	2.582(80)	2.574(44)	2.584(52)
P–O [Å]	1.5410(15)	1.544(15)	1.554(20)	1.533(22)	1.557(26)	1.516(44)	1.509(13)	1.482(42)	1.501(20)	1.497(22)
O–O in PO_4 [Å]	2.5316(30)	2.522(23)	2.597(42)	2.531(49)	2.567(96)	2.510(95)	2.437(28)	2.562(91)	2.477(40)	2.388(45)
O–P–O [deg]	110.5(1)	109.0(10)	109.0(1)	110.8(16)	109.0(10)	112.7(30)	108.3(10)	108.6(8)	111.2(15)	108.3(17)
θ [deg]	61.48	62.12	62.65	63.18	62.55	64.55	64.47	65.36	65.90	65.32
φ [deg]	0.313	0.868	1.232	1.193	1.548	1.982	2.004	2.118	2.656	3.256

Table 33A-1-023. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Average isothermal pressure derivatives of unit cell dimensions *a*, *c*, and of the structure parameters described in Table 33A-1-017. [a]) 0…1.65 GPa, [b]) 0…1.2 GPa, [c]) 0…1.1 GPa, [d]) 1.0…1.65 GPa [82 Tib], and [e]) 0…0.3 GPa [71Mor]. Neutron diffraction.

Derivative	Unit	KDP		DKDP	
		295 K	71 K	295 K	193 K
$\Delta a/\Delta p\|_T$	Å GPa^{-1}	−0.078(4) [a])	−0.084(5) [b])	−0.082(5) [a])	−0.090(6) [c])
		−0.058(8) [d])		−0.071(13) [d])	
		−0.096(2) [e])		−0.112(2) [e])	
$\Delta c/\Delta p\|_T$	Å GPa^{-1}	−0.072(5) [a])		−0.074(5) [a])	
		−0.065(8) [d])		−0.064(8) [d])	
		−0.073(2) [e])		−0.075(2) [e])	
$\Delta 2R/\Delta p\|_T$	Å GPa^{-1}	−0.015(5) [a])	−0.025(3) [b])	−0.021(2) [a])	−0.026(4) [c])
$\Delta\delta/\Delta p\|_T$	Å GPa^{-1}	−0.018(11) [a])	−0.040(8) [b])	−0.038(4) [a])	−0.038(6) [c])
$\Delta\theta/\Delta p\|_T$	deg GPa^{-1}	0.60(5) [a])	0.44(3) [b])	0.48(4) [a])	0.36(7) [c])

Table 33A-1-024. KH_2PO_4 (KDP), $KH_{2(1-x)}D_{2x}PO_4$ (x = 0.95). Degree of proton (deuteron) ordering, the displacement Δz(K) of K atom along the *z* axis relative to P atom, change in mean P–O distance Δ(P–O) from the value at Θ_f [85Nel]. P_s of KH_2PO_4 [73Sam] and $KH_{2(1-x)}D_{2x}PO_4$ [77Cha] are shown for comparison. Neutron diffraction.

T [K]	P_s [$\cdot 10^{-2}$ C m^{-2}]	H(D)-ordering [%]	Δz(K) [Å]	Δ(P–O) [Å]
KDP				
Θ_f – 1.3(3) K	3.25(15)	63.6(6)	0.0672(7)	0.0375(7)
Θ_f – 10(0.5) K	4.6(1)	86.8(8)	0.0970(7)	0.0532(7)
Θ_f – 20(1) K	4.85(5)	91.8(8)	0.1025(14)	0.0560(8)
DKDP (95% deuterated)				
Θ_f – 1.8(6) K	5.25(20)	84.6(4)	0.1149(14)	0.0600(10)
Θ_f – 5.8(6) K	5.80(5)	93.1(4)	0.1267(14)	0.0666(9)
Θ_f – 10(1) K	6.00(3)	96.0(2)	0.1298(7)	0.0693(6)

Table 33A-1-025. KD_2PO_4 (monoclinic DKDP). Fractional coordinates of atoms at RT in the monoclinic phase [75Tho]. Neutron diffraction.

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
K1	0.2312 (5)	0.1150 (1)	0.3664 (6)	O9	0.0565 (4)	0.4450 (3)	0.5316 (6)
K2	0.7184 (5)	0.1046 (3)	0.6593 (6)	O10	0.2062 (3)	0.2913 (3)	0.5308 (4)
K3	0.6253 (5)	0.4076 (3)	0.2086 (7)	O11	0.9813 (3)	0.3339 (3)	0.2747 (4)
K4	0.1436 (5)	0.3780 (3)	0.9266 (7)	O12	0.2795 (3)	0.4129 (3)	0.2939 (4)
P1	0.7374 (3)	0.1359 (3)	0.1766 (4)	O13	0.7234 (3)	0.4347 (3)	0.5833 (4)
P2	0.2274 (3)	0.1267 (3)	0.8682 (4)	O14	0.4861 (3)	0.4167 (3)	0.8220 (4)
P3	0.1408 (3)	0.3697 (2)	0.4069 (4)	O15	0.7807 (3)	0.3301 (3)	−0.1523 (4)
P4	0.6306 (3)	0.3726 (3)	0.7131 (4)	O16	0.5517 (4)	0.2879 (3)	0.6018 (5)
O1	0.8762 (3)	0.1696 (3)	0.3187 (4)	D1	0.5646 (4)	0.0163 (3)	0.2349 (5)
O2	0.6453 (3)	0.2123 (3)	0.0672 (5)	D2	0.9586 (5)	0.0664 (3)	0.0210 (6)
O3	0.5880 (3)	0.0814 (2)	0.2783 (4)	D3	0.4387 (5)	0.2060 (3)	0.0203 (6)
O4	0.8179 (3)	0.0658 (3)	0.0409 (5)	D4	0.1073 (4)	0.2220 (3)	0.6665 (5)
O5	0.1408 (3)	0.0556 (3)	−0.0125 (4)	D5	0.9221 (4)	0.4362 (3)	0.5519 (6)
O6	0.3667 (3)	0.0932 (3)	0.7429 (4)	D6	0.9397 (4)	0.2691 (3)	0.2984 (5)
O7	0.0669 (3)	0.1750 (3)	0.7551 (4)	D7	0.7358 (4)	0.2802 (3)	−0.0699 (5)
O8	0.3024 (5)	0.2054 (3)	0.0002 (5)	D8	0.4216 (5)	0.2897 (3)	0.5790 (6)

Table 33A-1-026. KH_2PO_4 (monoclinic). Fractional coordinates [95Mat]. T = 293 K. X-ray diffraction.

Atom	*x*	*y*	*z*
K(1)	0.5000	0.0544(1)	0.7500
K(2)	0.0000	0.3695(1)	0.2500
P(1)	0.5000	0.5721(1)	0.7500
P(2)	0.0000	–0.1127(1)	0.2500
O(11)	0.2748(2)	0.4479(2)	0.6144(2)
O(12)	0.5405(2)	0.6986(2)	0.6299(2)
O(21)	0.0818(2)	0.0144(2)	0.4128(2)
O(22)	–0.1982(2)	0.7702(2)	0.2060(2)
H(11)	0.309(5)	0.380(6)	0.714(4)
H(12)	0.441(4)	0.288(4)	0.023(3)

Table 33A-1-027. KH_2PO_4 (monoclinic). Anisotropic temperature parameters [$Å^2$] [95Mat]. T = 293 K. U_{ij} is defined by Eq. (d) in Introduction. X-ray diffraction.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
K1	0.0217(2)	0.0235(3)	0.0209(2)	0	0.0111(1)	0
K2	0.0229(2)	0.0225(3)	0.0389(2)	0	0.0162(1)	0
P2	0.0163(2)	0.0160(3)	0.0150(2)	0	0.0105(1)	0
P1	0.0194(2)	0.0210(3)	0.0178(2)	0	0.0107(1)	0
O11	0.0284(5)	0.0309(8)	0.0198(4)	–0.0130(5)	0.0126(3)	–0.0057(5)
O12	0.0211(4)	0.0285(8)	0.0196(4)	–0.0037(5)	0.0114(3)	0.0027(4)
O22	0.0280(4)	0.0318(7)	0.0208(4)	–0.0137(5)	0.0157(3)	–0.0054(5)
O21	0.0273(4)	0.0242(7)	0.0198(4)	–0.0071(5)	0.0163(3)	–0.0074(4)

Table 33A-1-028. KH_2PO_4 (monoclinic). Interatomic distances [Å] and angles [°] [95Mat]. T = 293 K. X-ray diffraction.

K ions			
K(1)–O(21$^{i, iii}$)	2.779(2)	K(2)–O(11$^{i, iii}$)	2.760(2)
K(1)–O(22$^{iv, v}$)	2.822(2)	K(2)–O(21$^{i, ii}$)	2.866(2)
K(1)–O(12$^{vi, vii}$)	2.907(2)	K(2)–O(12$^{x, xi}$)	2.915(2)
K(1)–O(11$^{i, iii}$)	3.160(2)	K(2)–O(22$^{viii, ix}$)	3.174(2)
Phosphate ions			
P(1)–O(11)	1.622(2)	P(2)–O(21)	1.553(2)
P(1)–O(12)	1.617(2)	P(2)–O(22)	1.525(2)
O(11)–P(1)–O(11^{iii})	122.44(9)	O(21)–P(2)–O(21^{ii})	107.04(9)
O(11)–O(1)–O(12)	108.31(9)	O(21)–P(2)–O(22)	109.31(9)
O(11)–P(1)–O(12^{iii})	108.54(9)	O(21)–P(2)–O(22^{ii})	109.42(9)
O(12)–P(1)–O(12^{iii})	110.72(9)	O(22)–P(2)–O(22^{ii})	112.19(9)
Hydrogen bonds			
O(11)–H(11)	0.94(3)	O(12)–H(12)	0.81(2)
H(11)...O(22)	1.79(4)	H(12)...O(22)	1.82(2)
O(11)...O(22)	2.614(2)	O(12)...O(22)	2.618(2)
O(11)–H(11)...O(22)	145(3)	O(12)–H(12)...O(22)	170(3)

Note. Symmetry operations: (i) x, y, z; (ii) $-x, y, ½ - z$; (iii) $1 - x, y, ½ - z + 1$; (iv) $-x, -y, 1 - z$; (v) $1 + x, -y, ½ + z, -1$; (vi) $x, y - 1, z$; (vii) $1 - x, y - 1, ½ - z + 1$; (viii) $x, 1 + y, z$; (ix) $-x, 1 + y, ½ - z$; (x) $1 - x, 1 - y, 1 - z$; (xi) $x - 1, 1 - y, ½ + z - 1$.

Table 33A-1-029. KDP family. Thermal expansion [67Coo].

Crystals	Sample length [mm]	Total contraction, 25 °C to Θ_f or Θ_{IV-III} $\Delta l/l$ [$\cdot 10^{-4}$]	Expansion coefficient α [$\cdot 10^{-6}$ K^{-1}]		Change of length at Θ_f or Θ_{IV-III} (on cooling) $\Delta L/L$ [$\cdot 10^{-4}$]	Change in volume at Θ_f or Θ_{IV-III} $\Delta V/V$ [$\cdot 10^{-4}$]
			Θ_f or Θ_{IV-III} to 25 °C	–50 °C to + 50 °C		
Along *a* axis						
KH_2PO_4	7.2	37.8	22.0	24.9	+5.5	+17.5
KD_2PO_4	4.9	15.1	19.4	20.1	+0.3	+10.5
KH_2AsO_4	5.2	34.2	17.5	24.2	+4.3	+15.1
KD_2AsO_4	6.5	18.3	12.9	15.1	+0.4, –1.9	+9.5...+4.9
RbH_2AsO_4	2.8	26.4	14.3	16.9	+7.5	+20.1
RbD_2AsO_4	2.4	14.5	11.2	14.3	+1.4	+9.8
$NH_4H_2PO_4$	7.3	40.8	27.2	32.0	+56	+42
$NH_4H_2AsO_4$	1.5	21.4	25.1	27.4	+56	+47.5
Along *c* axis						
KH_2PO_4	4.5	67.4	39.2	44.0	+6.5	
KD_2PO_4	3.9	29.6	39.5	40.7	+9.9	
KH_2AsO_4	5.8	83.6	43.6	47.1	+6.5	
KD_2AsO_4	5.0	61.5	43.3	45.6	+8.7	
RbH_2AsO_4	3.5	87.3	46.7	49.5	+5.1	
RbD_2AsO_4	2.5	61.4	47.3	49.5	+7.0	
$NH_4H_2PO_4$	6.1	16.2	10.7	4.2	–70	
$NH_4H_2AsO_4$	3.1	6.5	7.6	5.8	–64.5	

Table 33A-1-030. KD_2PO_4 (DKDP), RbH_2PO_4 (RDP), CsH_2PO_4 (CDP). Transition temperatures as functions of pressure [78Rap].

Phase boundary	Least-squares fit p in 10^8 Pa	Standard deviation K
RbH_2PO_4 II/I	$\Theta[°C] = 281 + 5.125p - 0.05715p^2$	1.7
RbH_2PO_4 V/I	$\Theta[°C] = 350 + 7.143\,(p-16.4) - 0.0919\,(p-16.4)^2$	1.9
RbH_2PO_4 V/Liquid	$\Theta[°C] = 402 + 3.909\,(p-24.4) - 0.0270\,(p-24.4)^2$	2.0
RbH_2PO_4 I/Liquid	$\Theta[°C] = 292.1 + 9.175p - 0.1955p^2$	1.9
CsH_2PO_4 II/I	$\Theta[°C] = 230 + 2.80p$	3.0
CsH_2PO_4 V/I	$\Theta[°C] = 262 + 8.716\,(p-11) - 0.1107\,(p-11)^2$	2.9
CsH_2PO_4 V/VI	$\Theta[°C] = 384.9 + 2.016\,(p-29.9)$	2.5
CsH_2PO_4 VI/I	$\Theta[°C] = 384.9 + 6.998\,(p-29.9) - 0.0828\,(p-29.9)^2$	2.0
CsH_2PO_4 VI/Liquid	$\Theta[°C] = 457 - 0.0411\,(p-42)$	0.7
CsH_2PO_4 I/Liquid	$\Theta[°C] = 345.7 + 8.340p - 0.1405p^2$	4.1
KD_2PO_4 I/Liquid	$\Theta[°C] = 250 + 7.334p - 0.1081p^2$	1.9
KD_2PO_4 VI/Liquid	$\Theta[°C] = 368.5 + 4.883\,(p-25) - 0.0724\,(p-25)^2$	1.4

Table 33A-1-031. KDP family. Parameters in the formula $E = (\varepsilon_0 C)^{-1} (T - \Theta_p) P + \xi P^3 + \zeta P^5 + \nu P^n$ [77Cha]. The content of deuterium in DKDP is about 70%.

Crystals	Θ_p [K]	C [$\cdot 10^3$ K]	ξ [$\cdot 10^{10}$ V m^5 C^{-3}]	ζ [$\cdot 10^{13}$ V m^9 C^{-5}]	n	ν
KH_2PO_4	122.76	2.9	2.57	5.95	11	$4.2 \cdot 10^{21}$ V m^{21} C^{-11}
KD_2PO_4	207.16	3.9	4.94	2.14	17	$9.9 \cdot 10^{27}$ V m^{33} C^{-17}
RbH_2PO_4	147.66	3.7	3.24	8.38	19	$1.94 \cdot 10^{32}$ V m^{37} C^{-19}
CsH_2AsO_4	146.15	2.9	9.18	6.13	15	$5.81 \cdot 10^{29}$ V m^{29} C^{-15}
KH_2AsO_4	96	2.49	17.0	6.54	29	$3.60 \cdot 10^{44}$ V m^{57} C^{-29}

Table 33A-1-032. KH_2PO_4 (KDP). C, ξ, ζ vs. p [78Wes]. Note the change of sign of ξ with the increase of pressure.

p [$\cdot 10^8$ Pa]	Sample no.	C [$\cdot 10^3$ K]	ξ [$\cdot 10^{10}$ V m^5 C^{-3}]	ζ [$\cdot 10^{13}$ V m^9 C^{-5}]
0.001	1	2.92(14)	–1.90(32)	4.3(11)
0.0016	2	3.20(6)	–1.20(4)	2.3(1)
0.001	3	3.21(3)	–1.02(4)	2.32(9)
1.00	2	3.45(8)	–0.72(4)	2.6(1)
2.00	3	3.22(16)	–0.52(5)	4.29(10)
2.40	3 (Run 1)	3.16(2)	–0.02(8)	3.1(2)
2.40	3 (Run 2)	3.31(4)	–0.25(29)	6.5(12)
2.40	3 (Run 3)	3.81(9)	+0.02(16)	3.2(4)
2.40	3 *)	3.23(3)	–0.02(5)	3.2(2)
3.00	2	3.11(8)	+0.73(4)	4.5(2)

*) Weighted average.

Table 33A-1-033. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Piezoelectric constants [66Bec].

Crystals	d_{14}	d_{36}	e_{36}	g_{14}	g_{36}	h_{14}	h_{36}	k_{36}	T	Ref.
	[$\cdot 10^{-12}$ CN^{-1}]		[Cm^{-2}]	[$\cdot 10^{-3}$ m^2 C^{-1}]		[$\cdot 10^{8}$ NC^{-1}]			[°C]	
KH_2PO_4(KDP)	1.28	20.9							20	38Spi
		21.7			112				27	56Bec
			0.142						20	50Van
				3.3	125	0.42	8.1		0	50Van
		16.8	0.097		110		6.48		100	46Mas
		18.0	0.104		112		6.63		80	
		19.7	0.117		116		6.96		60	
		21.1	0.127		116		7.05		40	
		23.2	0.142		118		7.32		20	
		25.4	0.158		119		7.50		0	
		28.6	0.180		121		7.68		–20	
		32.9	0.208		123		7.98		–40	
		39.7	0.252		125		8.19		–60	
		51.0	0.325		126		8.37		–80	
		67.3	0.427		127		8.43		–100	
		111	0.69		129		8.79		–120	
		160	0.97		130		8.91		–130	
		292	1.58		130		8.94		–140	
		488	2.33		131		9.06		–145	
		1470	4.3		132		9.21		–150	
KD_2PO_4(DKDP)		51.7							20	45Ban
		53.3							27	66Bec
		58.0			130			0.22	RT	63Sli

Table 33A-1-034. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Elastic compliances and stiffnesses.

Crystals	s_{11}	s_{12}	s_{13}	s_{33}	s_{44}	s_{66}	T	Ref.
	[$\cdot 10^{-11}$ m^2 N^{-1}]						[°C]	
KH_2PO_4	1.75	–0.4	–0.75	2.0	7.9	16.6	25	46Mas
(KDP)	1.53	0.2	–0.38	1.96	7.75	16.8	20	46Zwi
KD_2PO_4					7.77	16.1	RT	45Jaf
(DKDP)						16.5		50Jon
						17.1	27	56Bec
						16.5		63Sli
	1.575(8)	0.21(6)	–0.40(3)	2.014(8)	7.90(2)	16.83(4)	20	66Shu
	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}		
	[$\cdot 10^{10}$ N m^{-2}]							
KH_2PO_4	8.0	3.4	4.1	8.0	1.28	0.61	20	46Mas
(KDP)	6.91	–0.600	1.22	5.56	1.290	0.600	20	46Zwi
	7.14	–0.49	1.29	5.62	1.27	0.624		50Pri
	7.4	1.8	2.7	6.8	1.35	0.63		45Ban
	7.165	–0.627	1.494	5.640	1.248	0.621	20	64Hau
	7.17(3)	–0.63(9)	1.60(5)	5.68(3)	1.27(1)	0.64(2)		71Boy
KD_2PO_4	7.04	0.46				0.607	26	50Jon
(DKDP)	6.93	–0.78	1.22	5.45	1.265	0.594	20	66Shu

Table 33A-1-035. KH_2PO_4 (KDP). Refractive indices [64Zer]. T = 24.8 °C.

λ nm	Index in air		Absolute index	
	n_o	n_e	n_o	n_e
200	1.621996	1.563315	1.622630	1.563913
300	1.545084	1.497691	1.545570	1.498153
400	1.524035	1.479814	1.524481	1.480244
500	1.514498	1.472068	1.514928	1.472486
600	1.508851	1.467856	1.509274	1.468267
700	1.504817	1.465193	1.505235	1.465601
800	1.501508	1.463303	1.501924	1.463708
900	1.498514	1.461830	1.498930	1.462234
1000	1.495628	1.460590	1.496044	1.460993
1100	1.492730	1.459481	1.493147	1.459884
1200	1.489751	1.458443	1.490169	1.458845
1300	1.486645	1.457436	1.487064	1.457838
1400	1,483381	1.456437	1.483803	1.456838
1500	1.479938	1.455427	1.480363	1.455829
1600	1.476302	1.454395	1.476729	1.454797
1700	1.472459	1.453333	1.472890	1.453735
1800	1.468400	1.452234	1.468834	1.452636
1900	1.464118	1.451093	1.464555	1.451495
2000	1.459603	1.449906	1.460044	1.450308

Table 33A-1-036. KD_2PO_4 (DKDP). Refractive indices with respect to air [66Phi]. Accuracy: ±0.0001.

λ nm	Index at 298 K		Increase at 228 K	
	n_o	n_e	n_o	n_e
690.7	1.5022	1.4639	0.0019	0.0014
623.4	1.5044	1.4656	0.0020	0.0015
577.9	1.5063	1.4670	0.0019	0.0014
546.1	1.5079	1.4683	0.0020	0.0015
491.6	1.5111	1.4710	0.0020	0.0014
435.8	1.5155	1.4747	0.0020	0.0015
407.8	1.5185	1.4772	0.0020	0.0014
404.7	1.5189	1.4776	0.0020	0.0014

Table 33A-1-037. KH_2PO_4 (KDP). Ordinary (n_o) and extraordinary (n_e) refractive indices with respect to air [87Kir]. T = 33.0(4) °C.

λ [Å]	Source	n_o	n_e
4046.56	Hg	1.52322	1.47925
4358.33	Hg	1.51963	1.47635
4555.26	Cs	1.51779	1.47486
4678.15	Cd	1.51665	1.47386
4799.91	Cd	1.51570	1.47314
5085.92	Cd	1.51365	1.47150
5350.46	Tl	1.51195	1.47019
5460.74	Hg	1.51137	1.46983
5790.66	Hg	1.50970	1.46862
5893.0	Na	1.50897	1.46808
6438.47	Cd	1.50671	1.46644
7800.27	Rb	1.50201	1.46358
7947.60	Rb	1.50154	1.46328
8521.13	Cs	1.49975	1.46230
8943.46	Cs	1.49854	1.46173
10640.00	Xe	1.49383	1.45989

Table 33A-1-038. KD_2PO_4 (DKDP). Ordinary (n_o) and extraordinary (n_e) refractive indices with respect to air [87Kir]. T = 33.0(4) °C.

λ [Å]	Source	n_o	n_e
4046.56	Hg	1.51770	1.47696
4358.33	Hg	1.51427	1.47412
4678.15	Cd	1.51147	1.47174
4799.91	Cd	1.51055	1.47099
5085.82	Cd	1.50870	1.46945
5460.74	Hg	1.50662	1.46774
5893.0	Na	1.50472	1.46610
6438.47	Cd	1.50263	1.46449
7800.27	Rb	1.49882	1.46162
7947.60	Rb	1.49840	1.46146
8521.13	Cs	1.49721	1.46059
8943.46	Cs	1.49629	1.46007
10640.00	Xe	1.49314	1.45824

Table 33A-1-039. KH_2PO_4:Rb. Ordinary (n_o) and extraordinary (n_e) refractive indices with respect to air [87Kir]. T = 33.0(4) °C.

λ [Å]	Source	n_o	n_e
4046.56	Hg	1.52205	1.48070
4358.33	Hg	1.51858	1.47772
4678.15	Cd	1.51568	1.47534
4799.91	Cd	1.51470	1.47454
5460.74	Hg	1.51026	1.47107
5790.66	Hg	1.50866	1.46985
6438.47	Cd	1.50573	1.46780
7800.27	Rb	1.50103	1.46482
7947.60	Rb	1.50046	1.46453
8521.13	Cs	1.49883	1.46370
8943.46	Cs	1.49770	1.46311
10640.00	Xe +IF *)	1.49293	1.46117

*) To use a narrow bond interference filter.

Table 33A-1-040. KDP family. Coefficients for the two-resonance Sellmeier formula, $n^2 = 1 + [A\lambda^2/(\lambda^2 - B)] + [C\lambda^2/(\lambda^2 - D)]$ [87Kir]. $T = 33.0(4)$ °C. ord: ordinary ray, ext: extraordinary ray.

Crystal		A	B [$\cdot 10^{-10}$]	C [$\cdot 10^5$]	D
KH_2PO_4	ord	1.256618	0.84478168	33.89909	1.113904
	ext	1.131091	0.8145980	5.75675	0.8117537
KD_2PO_4	ord	1.239234	0.83531147	14.78889	0.8851187
	ext	1.125324	0.78980364	7.124567	1.190864
RbH_2PO_4	ord	1.250180	0.83869155	23.84257	0.8095880
	ext	1.159895	0.82190636	7.282928	0.9338123
RbD_2PO_4	ord	1.237455	0.82744984	17.69334	0.8839832
	ext	1.154309	0.81539261	5.85751	0.8927180
RbH_2AsO_4	ord	1.388219	1.1860891	31.01069	1.189864
	ext	1.274410	1.1267684	5.662958	1.147778
RbD_2AsO_4	ord	1.371661	1.1700309	16.30710	1.114844
	ext	1.269201	1.1202311	4.300136	1.149464
$NH_4H_2PO_4$	ord	1.298990	0.89232927	43.17364	1.188531
	ext	1.162166	0.85932421	12.01997	0.8318239
$ND_4D_2PO_4$	ord	1.278491	0.87627412	24.76201	1.196503
	ext	1.150918	0.84786983	7.611032	0.8107216
CsH_2AsO_4	ord	1.418170	1.2122778	25.12717	1.082196
	ext	1.349081	1.1927159	3.732809	0.8097333
CsD_2AsO_4	ord	1.405186	1.1903042	12.80897	0.8260685
	ext	1.343852	1.1821938	4.561628	1.191124
$NH_4H_2AsO_4$	ord	1.441185	1.2290244	30.08674	0.8843874
	ext	1.274199	1.1750136	11.96164	1.041567
$ND_4D_2AsO_4$	ord	1.418168	1.2246852	24.39162	1.175687
	ext	1.262361	1.1728953	6.250606	0.9188848
KH_2AsO_4	ord	1.411981	1.1955269	28.10751	1.006681
	ext	1.260916	1.1188613	5.258787	1.055210
KH_2PO_4:Rb	ord	1.253883	0.83916152	26.67790	0.8793790
	ext	1.134582	0.80876118	5.550476	0.8110137

Table 33A-1-041. KDP family. Coefficients for the modified Sellmeier formula, $n^2 = A + [CB/(C\lambda^2 - 1)] + [D\lambda^2/(E\lambda^2 - 1)]$ [87Kir]. T = 33.0(4) °C. ord: ordinary ray, ext: extraordinary ray.

Crystal		A	B [$\cdot 10^{-10}$]	C [$\cdot 10^{9}$]	D [$\cdot 10^{5}$]	E [$\cdot 10^{5}$]
KH_2PO_4	ord	2.257574	1.0115308	7.0637619	30.43721	17.27179
	ext	2.129495	0.96503229	72.513618	5.924875	7.870713
KD_2PO_4	ord	2.240921	0.96763930	6.4019860	17.70363	7.878938
	ext	2.126019	0.85784088	8.3393628	6.356423	8.103504
RbH_2PO_4	ord	2.249885	1.0559738	12.852642	28.99380	7.861649
	ext	2.159913	0.95146863	11.795379	7.740684	7.831282
RbD_2PO_4	ord	2.235596	1.092894	72.513815	18.56709	7.883038
	ext	2.152727	1.0022483	72.509186	5.442314	7.873119
RbH_2AsO_4	ord	2.390661	1.5512827	5.5211018	27.50904	7.888619
	ext	2.275570	1.3914908	6.8528051	5.686596	7.896969
RbD_2AsO_4	ord	2.373255	1.5429898	6.3143511	15.58845	7.874832
	ext	2.270806	1.3592076	6.2632863	4.740838	17.21615
$NH_4H_2PO_4$	ord	2.301929	1.0569191	5.6024115	38.10084	21.37123
	ext	2.162273	0.98656652	9.6615997	14.23869	7.807344
$ND_4D_2PO_4$	ord	2.279481	1.0760835	7.5398211	20.97227	17.24865
	ext	2.151161	0.96521770	10.296373	9.470799	7.898857
$C_5H_2AsO_4$	ord	2.420405	1.6272261	5.5538145	24.26902	17.29381
	ext	2.350262	1.5645403	6.7472517	5.384884	7.857386
$C_5D_2AsO_4$	ord	2.408170	1.5597934	5.2351416	17.43638	7.882014
	ext	2.345809	1.5141459	5.9396419	5.119295	7.853574
$NH_4H_2AsO_4$	ord	2.443449	1.6756541	5.4726728	34.88801	17.29053
	ext	2.275962	1.4296386	6.0383457	12.59613	7.881151
$ND_4D_2AsO_4$	ord	2.413739	1.9040362	41.206727	17.41336	16.79311
	ext	2.259082	1.6092255	38.009278	4.502676	24.05449
KH_2AsO_4	ord	2.414647	1.5841464	5.3694136	29.49448	7.880000
	ext	2.262579	1.3461143	6.1858412	6.054821	7.870687
KH_2PO_4:Rb	ord	2.253999	1.0418508	10.184912	30.14009	7.897699
	ext	2.134917	0.90364403	10.257328	7.006997	7.530137

Table 33A-1-042. KH_2PO_4 (KDP), RbH_2PO_4 (RDP), $NH_4H_2PO_4$ (ADP). $\partial n/\partial T$ of phosphates for several λ in the range from 20 °C to 50 °C [82Bar]. o: ordinary ray, e: extraordinary ray.

	Ray	$\partial n/\partial T$ [K^{-1}]				
		λ [μm]	0.633	0.578	0.546	0.436	0.405
KH_2PO_4	o		−39.4	−32.5	−32.8	−32.7	−32.7
	e		−25.4	−28.7	−29.0	−28.8	−31.5
KD_2PO_4	o		−31.6	−30.0	−29.9	−33.7	−30.0
	e		−20.3	−25.2	−19.5	−21.3	−18.6
RbH_2PO_4	o		−37.2	−37.2	−37.2	−38.6	−36.9
	e		−28.9	−28.0	−25.4	−27.6	−26.7
$NH_4H_2PO_4$	o		−50.8	−46.0	−52.3	−49.4	−47.8
	e		0.0	0.0	0.0	0.0	0.0

Table 33A-1-043. KH_2PO_4:Tl, RbH_2PO_4:Tl. Position, FWHM, intensity ratio of absorption band determined as the integrated absorption strength of the band relative to that of the A_z band at LNT [94Fuj]. See Fig. 33A-1-156 for absorption bands A_z, etc. Values in parentheses of A_{xy} bands stand for the doublet components.

	Absorption band		A_z	A_{xy}	B_{xy}	C_{xy}	C_z
KDP:Tl	Position (eV)	RT	5.53	5.73(5.63, 5.78)	6.88		
		LNT	5.56	5.76(5.68, 5.81)	6.91	7.30	7.67
	FWHM (eV)	RT	0.21	(0.20, 0.16)	0.19		
		LNT	0.10	(0.14, 0.12)	0.09	0.26	0.22
	Intensity ratio	RT	1.00	1.28(0.59, 0.69)	2.35		
		LNT	1.00	1.22(0.56, 0.66)	1.85	8.0	9.8
RDP:Tl	Position (eV)	RT	5.55	5.72(5.64, 5.80)	6.90		
		LNT	5.58	5.80(5.72, 5.84)	6.96	7.35	
	FWHM (eV)	RT	0.21	(0.26, 0.16)	0.2		
		LNT	0.12	(0.18, 0.10)	0.12	0.34	
	Intensity ratio	RT	0.80	1.48(0.74, 0.74)	3.6		
		LNT	1.00	1.62(0.76, 0.86)	1.7	6.9	

Table 33A-1-044. KH_2PO_4 (KDP). Frequencies ω [cm^{-1}] and TO oscillator strength $\Delta\kappa$ of A_1 modes determined from far-infrared reflectivity [92Bre]. T = 7 K.

ω_{TO} [cm^{-1}]	ω_{LO} [cm^{-1}]	$\Delta\kappa$
172	177	0.80
213.5	245	2.93
248	285	0.14
345.5	374	0.35
462	474	0.13
511	524	0.09

Table 33A-1-045. KD_2PO_4 (DKDP). Frequencies ω [cm^{-1}] of the far-infrared active modes along the c axis [88Bre]. T = 293 K (paraelectric phase, B_2 modes) and T = 7 K (ferroelectric phase, A_1 modes). T, L and ν_i refer to the expected translational, librational and internal modes, respectively.

Numbering of the modes		PE phase			FE phase	
n		ω_{TO} [cm^{-1}]	ω_{LO} [cm^{-1}]		ω_{TO} [cm^{-1}]	ω_{LO} [cm^{-1}]
1		2.2				
2	T	156.5	157	L	161	170.5
3	T	182	199	T	214.5	218
4	T	222	268	T	225	274
5	ν_2	344	354	ν_2	346	362
6	ν_2	386	389	ν_2	380	385
7	ν_4	475	505	ν_4	496	500
				ν_4	508	519

Table 33A-1-046. KD_2PO_4 (DKDP). Frequencies ω [cm^{-1}] of the far-infrared active modes in a direction perpendicular to the *c* axis [88Bre]. T = 293 K (paraelectric phase, E modes) and T = 7 K (ferroelectric phase, B_1 or B_2 modes). ν_4: 4th internal mode.

Numbering of the modes n		PE phase		FE phase		
		ω_{TO} [cm^{-1}]	ω_{LO} [cm^{-1}]	ω_{TO} [cm^{-1}]	ω_{LO} [cm^{-1}]	Assignment
1	Lattice modes	22.5	42.5			
2		98	100	96	96.25	B_1
				103	104	B_2
3		107	110	116.25	117	B_2
				120	120.5	B_1
4		123.5	130	132	142	B_2
5		183	195	178	179	B_2
				189	201	B_1
				213	214	B_1
6		219	273	225	250	
				263	293	B_2
7	ν_4	375	410	415	416	
8		450	470	452	468	B_2
9		532	555	518	535	B_2
				540	555	B_1

Table 33A-1-047. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Electrooptic constants.

Crystals	r_{41}^T	r_{41}^S	r_{63}^T	r_{63}^S	ρ_{63}^T	T [°C]	λ [nm]	Ref.
	[$\cdot 10^{-12}$ m V^{-1}]				[$\cdot 10^{-3}$ m^2 C]			
KH_2PO_4(KDP)	8.6		+10.5			22	556	50Car
			–11.6			20	546	44Zwi
	8.8		10.3			RT	546	64Ott
			12.0	3.5				63Mye
			9.7					53Car
			10.0				546.1	61Nam
					–62.7			44Zwi, 50Bec
			9.7					64Van1
				8.3			400…725	66Vas
				8.8			633	67Ros
			9.4	8.15			633	67Ohm
	8.5			9.3			633	76For
	–8.28	–8.25	10.22	8.89		21	589	78Vee
KD_2PO_4 (deuterated KDP)			–23.3			RT		59Jaf
			–26.4			RT	546	63Sli
			–20			20	546	44Zwi
					–41.7			44Zwi, 50Bec
83…92% deuterated KDP	8.8							64Ott

Table 33A-1-048. KDP family. ρ_{63} vs. T [71Vas]. ρ_{63}: electrooptic constant for ***P***. λ = 535 nm.

Crystals	ρ_{63}							
	[$\cdot 10^{-2}$ m^2 C^{-1}]							
	20 °C	0 °C	–20 °C	–40 °C	–60 °C	–80 °C	–100 °C	–120 °C
KH_2PO_4(KDP)	5.7	6.3	6.6	6.9	6.9	6.9	6.9	6.9
KD_2PO_4(DKDP)	5.7	6.0	6.0	6.0				
RbH_2PO_4(RDP)	5.7	6.0	6.3	6.6	6.6	6.6		
KH_2AsO_4(KDA)	6.9	7.2	7.5	7.8	7.8	7.8	7.8	7.8
RbH_2AsO_4(RDA)	6.6	6.9	7.5	7.8	8.1	8.4	8.4	8.4
CsH_2AsO_4(CDA)	7.5	8.1	8.4	8.7	8.7	8.7	8.7	8.7

Table 33A-1-049. $KH_{2(1-x)}D_{2x}PO_4$. $r_{i\lambda}$ vs. x [73Vol]. $r_{i\lambda}$: electrooptic constants.

x	r_{63} [$\cdot 10^{-12}$ m V^{-1}]	r_{41} [$\cdot 10^{-12}$ m V^{-1}]
0	9.9(2)	8.6(2)
0.18	10.1(3)	
0.30	11.7(3)	
0.40	13.4(4)	
0.50	12.8(4)	9.3(3)
0.70	16.0(6)	
0.86	19.8(7)	10.7(3)
0.90	22.7(12)	10.9(3)
0.96	23.3(12)	
0.98	25.8(2)	10.7(3)
0.998	26.4(7)	

Table 33A-1-050. KH_2PO_4 (KDP). Piezooptic constants. $\Pi_{\lambda\mu}$: piezooptic constant for **T**. $p_{\lambda\mu}$: piezooptic constant for **S**.

$\Pi_{11}-\Pi_{12}$	Π_{11}	Π_{12}	Π_{13}	Π_{31}	Π_{33}	Π_{44}	Π_{66}	λ	Ref.
[$\cdot 10^{-12}$ m^2 N^{-1}]								[nm]	
> –0.3, < 0							–11.25 (Π_{66}^E)	560	50Wes
							–8.6 (Π_{66}^E)		59Jaf
	4.15	4.08	1.12	3.60	0.44	–1.47	–10.26	589	75Vee
3 *)							10 *)		76Sav
$p_{11}-p_{12}$	p_{11}	p_{12}	p_{13}	p_{31}	p_{33}	p_{44}	p_{66}		
dimensionless									
> –0.7, < 0							–6.85 (p_{66}^E)	560	50Wes
	0.251 *)	0.249 *)	0.246 *)	0.225 *)	0.221 *)		0.058 *) (p_{66}^E)	633	67Dix
	0.25 *)	0.259 *)		0.219 *)				633	73Mar
	0.287	0.282	0.174	0.241	0.122	–0.019	–0.064	589	75Vee
	0.254 *)	0.230 *)	0.233 *)	0.221 *)	0.212 *)			633	77Ale

*) Absolute value.

Table 33A-1-051. KH_2PO_4 (KDP), KD_2PO_4 (DKDP), RbH_2PO_4 (RDP). $p_{\lambda\mu}$: piezooptic constants for **S** [83Ava]. Δp_{44}: antisymmetric tensor component (rotooptic constant).

	KH_2PO_4(KDP)	KD_2PO_4(DKDP)	RbH_2PO_4(RDP)
p_{11}	+0.238	+0.241	+0.247
p_{12}	+0.249	+0.247	+0.265
p_{13}	+0.242	+0.245	+0.248
p_{33}	+0.242	+0.245	+0.248
p_{31}	+0.227	+0.236	+0.229
p_{44}	−0.034	−0.035	−0.032
p_{66}	−0.068	−0.072	−0.032
Δp_{44}	0.0127	0.0125	0.0095

Table 33A-1-052. KH_2PO_4 (KDP), KD_2PO_4 (DKDP; tetragonal, monoclinic). Activation energy ΔU of the electric conductivity along the *c* axis. Estimated from the conductivity vs. *T* curves, $\sigma \propto \exp(-\Delta U/kT)$.

Crystals	Temperature range	ΔU [eV]	Ref.
KH_2PO_4 (tet.)	$T < \approx 180$ °C	0.543(5)	67OKe1
	$T > \approx 180$ °C	0.78(7)	67OKe1
KD_2PO_4 (tet.)	$T < \approx 102$ °C	0.53(1)	67OKe1
	$T > \approx 102$ °C	0.82(4)	67OKe1
KD_2PO_4 (mon.)	$T > 563$ °C	0.47(4)	88Yak

Table 33A-1-053. KH_2PO_4 (KDP). $\langle \Delta\nu^2 \rangle^{1/2}$ of proton resonance [62Bjo].

	$\langle \Delta\nu^2 \rangle^{1/2}$ (exp)	$\langle \Delta\nu^2 \rangle^{1/2}$ (calc)
H along *c*	5.2 kHz	4.6 kHz
H along *a*	5.6	5.3

Table 33A-1-054. KD_2PO_4 (DKDP), KD_2AsO_4 (DKDA), CsD_2AsO_4 (DCDA). Principal values, eigenvectors and angles between the X-bond deuteron quadrupole coupling tensor eigensystem and the *X*(*a*), *Y*(*b*), *Z*(*c*) crystal axes system [71Bli2].

		$(eQ/h)\phi_{zz}$[kHz]			$(eQ/h)\phi_{yy}$[kHz]			$(eQ/h)\phi_{xx}$[kHz]	
KD_2PO_4									
	T= 30 °C		119.7			−62.6			−56.9	
		±1	0	0	0	0	±1	0	±1	0
		0°	90°	90°	90°	90°	0°	90°	0°	90°
	T= −100 °C		127.5			−71.1			−56.4	
		±1	0	0	0	±0.58	0.81	0	0.81	±0.58
		0°	90°	90°	90°	55°	±35°	90°	±35°	55°
KD_2AsO_4										
	T= 30 °C		118.5			−62.0			−55.9	
		±0.99	0	±0.04	±0.04	0	±0.99	0	±1	0
		2°	90°	88°	88°	90°	2°	90°	0°	90°
	T= −123 °C		125.1			−65.4			−54.6	
		±0.99	0.02	∓0.030	±0.04	±0.55	0.82	0	0.83	±0.55
		2°	88°	88°	88°	56°	±34°	90°	±34°	56°
CsD_2AsO_4										
	T= 30 °C		121.5			−64.0			−57.5	
		±1	0	0	0	0	±1	0	±1	0
		0°	90°	90°	90°	90°	0°	90°	0°	90°
	T= −68 °C		126.7			70.0			−54.0	
		±1	0	0	0	∓0.54	0.84	0	0.84	∓0.54
		0°	90°	90°	90°	57°	±33°	90°	±33°	57°

Table 33A-1-055. KH_2PO_4 (KDP). ^{39}K electric field gradient tensor components at 77 K [68Tsu]. There are two non-equivalent sites A and B for K in a unit cell (see illustration in 3b). *X, Y, Z* axes are the tetragonal *a, b, c* axes in the paraelectric phase.

	$eQ\phi_{zz}/12\,h$ [kHz]	$eQ\phi_{yy}/12\,h$ [kHz]	$eQ\phi_{xx}/12\,h$ [kHz]	$eQ\phi_{xy}/12\,h$ [kHz]
Site A	123.3(7)	− 19.3(12)	–104.0(18)	7.1(33)
Site B	123.3(7)	–104.0(12)	− 19.3(12)	7.1(33)

Table 33A-1-056. KH_2PO_4 (KDP), KD_2PO_4 (DKDP), $NH_4H_2PO_4$ (ADP). Principal values of ^{31}P chemical shift tensor. $\Delta\sigma = \sigma_{\parallel} - \sigma_{\perp}$, $\bar{\sigma} = (\sigma_{\parallel} + 2\sigma_{\perp})/3$, $\sigma_{\parallel}$, $\sigma_{\perp}$: components parallel or perpendicular to the *c* axis.

	$\sigma_{\parallel}$	$\sigma_{\perp}$	$\Delta\sigma$	$\bar{\sigma}$	T	Ref.
KH_2PO_4	– 1.1	–16.5	15.4	–11.2	77 K	74Ter
KH_2PO_4	12.8(2)	–14.7(2)	27.5	– 5.5	RT	
KD_2PO_4	12.8(2)	–13.1(2)	25.9	– 4.5	RT	76Jas
$NH_4H_2PO_4$	20.0(2)	–12.5(2)	32.5	– 1.5	RT	

Table 33A-1-057. KH_2PO_4 (KDP). EFG tensor parameters for ^{17}O, and O–H bond distance and bond direction determined from the NQR data [81Bro]. θ and ϕ are polar angles in the EFG principal axial system, η: asymmetry parameter. A, B: ferroelectric oxygen sites, C: paraelectric oxygen site.

Sites	Temperature [K]	e^2qQ/h [kHz]	η	$eQ\phi_{zz}/h$ [kHz]	$eQ\phi_{yy}/h$ [kHz]	$eQ\phi_{zz}/h$ [kHz]	O–H distance [nm]	θ [°]	ϕ [°]
A (P–O–H)	77	−5845(5)	0.718(3)	−5845(5)	+5021(15)	824(10)	0.105(1)	45(10)	0(20)
B (P=O)	77	±4690(10)	0.31(2)	∓4690(10)	±3072(30)	±1618(25)	–	–	–
C (P–O)	160	−5115(5)	0.572(3)	−5115(5)	+4020(10)	+1094(10)	0.119(2)	50(10)	0(20)

Table 33A-1-058. KH_2PO_4 (KDP), CsH_2PO_4 (CDP). ^{17}O quadrupole coupling constants and asymmetry parameters [86Bli].

System		e^2qQ/h [kHz]	η
I. KH_2PO_4			
$T > \Theta_f$			
Disordered		–5115(5)	0.572(3)
$T < \Theta_f$			
Close	^{17}O–H…O	–5845(5)	0.718(3)
Far	^{17}O…H–O	–4690(10)	0.310(2)
II. CsH_2PO_4			
$T > \Theta_f$			
Ordered	^{17}O–H(1)…O	6500	0.75
Disordered	^{17}O–H(2)…O	5300	0.57
$T < \Theta_f$			
	^{17}O–H(1)…O	6500	0.75
Close	^{17}O–H(2)…O	6100	0.70
Far	^{17}O…H(2)–O	4600	0.30

Table 33A-1-059. KH_2PO_4:VO^{2+}. Spin Hamiltonian parameters for VO^{2+} in KH_2PO_4 at RT [78Koh]. A: in the unit of 10^{-2} m^{-1}. θ, ϕ: direction of the symmetry axis (V–O bond) relative to the tetragonal axis. Three distinct hyperfine patterns of different intensity were observed corresponding to three chemically distinct sites I, II, III.

Parameters	Site I	Site II	Site III
$g_{\parallel}$	1.924(1)	1.929(2)	1.933(2)
$g_{\perp}$	1.975(2)	1.982(2)	1.985(2)
$A_{\parallel}$	182.0(5)	177.1(10)	180.8(10)
$A_{\perp}$	70.9(10)	68.1(10)	68.9(20)
θ	18.5(10)°	90(1)°	34(10)°
ϕ	20(2)°	20(2)°	36(10)°
Intensity	15	2	1

Table 33A-1-060. KH_2PO_4 (KDP). ESR data [67Sar, 69Ota]. Direction cosines x_i, y_i, z_i of principal axes of **g** and **A** tensors for Mn^{2+} center relative to the crystallographic axes a, b, c are indicated.

Paramagnetic center	Site	S	**H**	ν [GHz]	T [K]	g-factor	HF $\lvert^{n}A\rvert$ [$\cdot 10^{-2}$ m^{-1}]
Mn^{2+}	*)	5/2	(6)	9.5	RT	$g_{x_1} = 0.63(1)$	$\lvert^{55}A_{z_1}\rvert = 95$
[67Sar]						$g_{y_1} = 0.98$	
						$g_{z_1} = 2.2$	
						$g_{x_2} = 0.70$	$\lvert^{55}A_{z_2}\rvert = 75$
						$g_{y_2} = 1.07$	
						$g_{z_2} = 3.5$	
						$g_{x_3} = 0.54$	$\lvert^{55}A_{x_3}\rvert = 70(10)$
						$g_{y_3} = 1.01$	$\lvert^{55}A_{y_3}\rvert = 70(10)$
						$g_{z_3} = 2.28$	$\lvert^{55}A_{z_3}\rvert = 110(5)$
Cu^{2+}	**)	1/2		≈ 9	109	$g_{\parallel} = 2.364$	$A_{\parallel} = 142$
[69Ota]						$g_{\perp} = 2.080$	$A_{\perp} = 19$
						$g_{\parallel} = 2.340$	$A_{\parallel} = 145$
						$g_{\perp} = 2.072$	$A_{\perp} = 20$

*) Mn^{2+} ions are shown to be located on three nonequivalent sites, with C_2 symmetry.
**) Two different K^+ sites accompanied by vacancies.

	x_1	y_1	z_1	x_2	y_2	z_2	x_3	y_3	z_3
a	0.951	0.309	0	0.766	0.643	0	0.985	0.174	0
b	0.309	0.951	0	0.643	0.766	0	0.174	0.985	0
c	0	0	1	0	0	1	0	0	1

Table 33A-1-061. KH_2PO_4 (KDP). **A** and **g** tensor of KH_2PO_4:Tl^{2+} centers [82Gon]. Direction cosines refer to the (a*, b, c) frame.

	Principal values		Direction cosines
	g	A [MHz]	(λ, μ, ν)
295 K	1.990	115660	X: (0, 0, 1)
	1.995	116150	Y, Z: (λ, μ, 0)
77 K	1.987	115660	X: (0, 0, 1)
(A_+)	1.995	116135	Y: (0.917, –0.399, 0)
	2.000	116680	Z: (0.399, 0.917, 0)
4.2 K	1.988	114322	X: (0.291, –0.0251, 0.956)
(A'_+)	1.994	114900	Y: (0.859, –0.432, –0.273)
	2.001	115560	Z: (0.420, 0.901, –0.104)

Table 33A-1-062. KD_2PO_4 (DKDP). **A** and **g** tensor of KD_2PO_4:Tl^{2+} centers [83Gon]. Direction cosines refer to the (a, b, c) frame. T = 240 K.

Centers	g	A [MHz]	Direction cosines (λ, μ, ν)
I	1.990	116338	X: (0, 0, 1)
	1.995	116850	Y, Z: (λ, μ, 0)
II	1.981	101846	X: (0.212, –0.149, 0.966)
	1.990	102699	Y: (0.826, –0.501, –0.258)
	1.998	103600	Z: (0.522, 0.852, –0.018)
III	1.985	107959	X: (+0.117, +0.043, 0.992)
	1.998	108479	Y: (0.702, –0.710, –0.052)
	1.995	108954	Z: (0.703, 0.703, –0.113)

Table 33A-1-063. KH_2PO_4 (KDP):Fe^{3+}. Principal values and direction cosines of fine structure **D** tensor [76Tsu]. D_{ii} in the unit of 10^3 A m^{-1}.

Principal values		Direction cosines		
		λ	μ	ν
D_{xx}	41.9(4)	0.628	0.739	0.243
D_{yy}	–38.3(4)	0.761	–0.649	0.003
D_{zz}	– 3.6(4)	–0.160	–0.183	0.970

Table 33A-1-064. KH_2PO_4:Cr^{3+}. Proton hyperfine tensor decomposed in the isotropic (A_{iso}) and anisotropic (B_{ii}) parts determined by ENDOR at 4.2 K [92Bra]. θ, φ: polar and azimuthal angles in the crystal axis (a, b, c) system.

Proton	A_{iso}	B_{ii}, $i = x, y, z$	θ	φ
	[MHz]	[MHz]	[°]	[°]
1	3.39(9)	–5.12(12) –4.67(8) 9.79(8)	83 107 19(1)	232 320 342(2)
2	2.41(12)	–4.11(9) –3.80(15) 7.91(12)	63 148 105(2)	74 40 156(1)
3	2.13(44)	–4.21(80) –4.80(25) 9.01(29)	101 73 20(1)	215 302 158(2)
4	5.58(26)	–7.21(15) –1.14(47) 8.35(17)	58 120 134(3)	276 206 329(1)
5	–1.00(16)	–4.01(30) –0.30(12) 4.31(11)	86 35 125(2)	342 246 255(2)
6	0.60(14)	–1.78(10) –1.31(7) 3.09(3)	151 98 62(3)	192 297 212(3)

Table 33A-1-065. KH_2PO_4:Cr^{3+}. Directions and distances of $K^+ - H^+$ determined by ENDOR of Cr^{3+} ion of K^+ position [92Bra]. θ, φ: polar and azimuthal angles in the crystal axis (a, b, c) system. A_Z, A'_Z, C_Z, C'_Z : nearest protons of K^+ ion. A_Y, A'_Y, C_Y, C'_Y : next nearest protons of K^+ ion.

Proton	K^+–H^+ direction		K^+–H^+ distance
	θ [°]	φ [°]	[Å]
A_Z	140.2(1)	59.4(1)	
A'_Z	140.2(1)	239.4(1)	3.38(1)
C_Z	39.8(1)	149.4(1)	
C'_Z	39.8(1)	329.4(1)	
A_Y	74.8(1)	35.4(1)	
A'_Y	74.8(1)	215.4(1)	3.32(1)
C_Y	105.2(1)	125.4(1)	
C'_Y	105.2(1)	305.4(1)	

Table 33A-1-066. KH_2PO_4: SeO_4^{3-}, KH_2PO_4: AsO_4^{4-}. Proton hyperfine splitting tensor components [in MHz] and the associated direction cosines measured by ENDOR [94Rak1].

	Isotropic	Anisotropic	λ	μ	ν
SeO_4^{3-}					
		23.71	–0.0662	–0.9932	0.0955
"Close" proton [a])	–17.71	–3.02	0.9772	–0.0451	0.2076
		–20.69	0.2018	–0.107	–0.9166
		1.31	0.203	0.7881	0.5811
"Far" proton [b])	0.25	–0.5	–0.3998	0.6084	–0.6855
		–0.81	0.8938	0.0931	–0.4386
AsO_4^{4-}					
		22.84	–0.075	–0.994	0.0752
"Close" proton [c])	–13.6	–3.15	0.9183	–0.0314	0.392
		–19.69	0.3871	–0.0982	–0.9166
		5.09	0.4063	0.7086	0.5769
"Far" proton [c])	–2.83	–0.37	–0.538	0.6958	–0.4758
		–4.73	0.7386	0.1171	–0.6639

Taken from references: [a]) [77Dal], [b]) [94Rak1], [c]) [72Dal]

Table 33A-1-067. KH_2PO_4: SeO_4^{3-}. Superhyperfine coupling tensor measured by ENDOR. T = 4.2 K. θ, φ: polar and azimuthal angle in the crystal axis (a, b, c) system. The data for the close protons, A^{close}, are from [77Dal], and those for the far protons, A^{far}, are from [92Rak1].

Tensor component	Principal value [MHz]	θ [°]	φ [°]
A_x^{close}	6.00(3)	84	94
A_y^{close}	–20.73(3)	78	2
A_z^{close}	–38.40(3)	13	–152
A_x^{far}	≈ |2|		
A_y^{far}	≈ |1|		
A_z^{far}	≈ |1|		

Table 33A-1-068. KH_2PO_4: AsO_4^{4-}, KH_2AsO_4. Superhyperfine coupling tensor measured by ENDOR for AsO_4^{4-} [89Dal2]. $\boldsymbol{H} \parallel \boldsymbol{c}$. T = 103 K.

Compound	Nucl.	$A_\parallel$ [MHz]	$A_\perp$ [MHz]	Q [MHz]
KH_2AsO_4	^{39}K	4.84(2)	2.59(40)	0.23(3)
KH_2PO_4	^{39}K	6.08(2)	3.17(40)	0.25(3)
KH_2PO_4	^{31}P	1.61(2)	–	–

Table 33A-1-069. KH_2PO_4: CrO_4^{2-}, $NH_4H_2PO_4$: CrO_4^{2-}. Principal values of *g*-factor and their direction cosines of crystals γ-irradiated at RT [93YuJ]. *T* = RT.

Host	Species	Principal *g*-values	Direction cosines λ	μ	ν
KH_2PO_4	A	2.046	[–0.422,	0.891,	0.168]
		2.007	[0.654,	0.171,	0.737]
		2.004	[0.628,	0.421,	–0.655]
	B	2.040	[–0.548,	0.754,	0.364]
		2.007	[0.001,	–0.433,	0.902]
		2.002	[0.837,	0.494,	0.237]
$NH_4H_2PO_4$		2.041	[0.518,	0.775,	0.362]
		2.008	[0.007,	–0.428,	0.904]
		2.003	[0.856,	–0.465,	–0.227]

Table 33A-1-070. KH_2PO_4 (KDP). Diagonal **g** tensor values and their direction cosines for ESR measurememt [86Wel]. Specimens are X-ray irradiated at 4.2 K and 77 K. Direction cosines of O–O and P–O in a PO_4 group from low temperature structure data are also indicated.

g value	λ	μ	ν
4.2 K species			
2.0184	0.43	0.90	0
2.0177	0	0	1
2.0096	0.90	–0.43	0
Structure data			
O_1–O_2	0.48	0.88	0
O_3–O_4	0.88	–0.48	0
77 K species			
2.0487	0.21	0.78	0.58
2.0071	–0.41	–0.47	0.78
2.0037	0.89	–0.41	0.21
Structure data			
P–O_1	0.39	0.71	0.58
P–O_1×P–O_2	0.88	–0.48	0

Table 33A-1-071. KH_2PO_4 (KDP). Proton hyperfine splitting tensors and associated direction cosines for ENDOR measurements [86Wel]. Specimens are X-ray irradiated at 4.2 K and 77 K. Iso.: isotropic component. Aniso.: anisotropic component. Direction cosines of O–H bonds from low temperature structure data are also indicated.

	Proton hyperfine splitting tensors [MHz]			
Iso.	Aniso.	λ	μ	ν
4.2 K species				
	+14.17	0.99	–0.02	–0.05
–1.03	–8.15	0.05	0.40	0.92
	–6.02	0.0	0.92	–0.40
Structure data				
	O_1–H_1	0.999	0	0.03
77 K species				
Proton 1				
	+8.52	–0.39	0.75	–0.54
+0.33	–1.35	0.52	0.66	0.54
	–7.17	0.76	–0.07	–0.65
Structure data				
	O_1–H_4	–0.67	0.35	–0.66
Proton 2				
	+4.33	–0.15	0.98	0.14
–0.55	–1.91	–0.06	–0.15	0.99
	–2.42	0.99	0.14	0.08
Structure data				
	O_3–H_3	0	–0.999	–0.03

Table 33A-1-072. KH_2PO_4 (KDP). Hyperfine splitting tensors of P and associated direction cosines for ENDOR measurements [86Wel]. Specimens are X-ray irradiated at 4.2 K and 77 K. Iso.: isotropic component. Aniso.: anisotropic component. Direction cosines of O–O and P–O in a PO_4 group from low temperature structure data are also indicated.

	Phosphorous hyperfine splitting tensors [MHz]			
Iso.	Aniso.	λ	μ	ν
4.2 K species				
	–3.31	0	0	0
–82.21	–0.23	0.35	0.94	0
	+3.54	0.94	–0.35	0
Structure data				
	O_1–O_2	0.48	0.88	0
	O_3–O_4	0.88	–0.48	0
77 K species				
	–3.97	0.82	–0.57	0.03
–89.77	0.82	0.46	0.69	0.57
	+3.15	–0.34	–0.45	0.82
Structure data				
	P–O_1	0.39	0.71	0.58
	P–O_1×P–O_2	0.88	–0.48	0

Table 33A-1-073. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Components of the ferroelectric eigenvector in units of 10^{-3} Å just above Θ_f [86And]. K_z means the z-component of eigenvector for K, and so on. Δ_z: z-component of eigenvector for the center of gravity. Values are determined by the use of X-ray diffuse scattering intensity. O_c of DKDP in the refinement was held fixed at the reported value of 0.037 Å [80Hos].

	X-rays		Neutron data
	KDP	DKDP	DKDP
K_z	10.3(8)	11.7(11)	7(10)
P_z	–51.0(10)	–80(16)	–83(8)
O_z	–21.2(12)	–18.3(18)	–22(3)
O_b	–5.3(29)	–10.4(25)	–1(2)
O_c	–41(44)	37	37
Δ_z	–19	–24	–27

Table 33A-1-074. KH_2PO_4 (KDP), KD_2PO_4 (DKDP). Peak energies E and full width at half-maximum Γ of vibrational modes of H(D) atom and PO_4 group obtained from neutron incoherent scattering and Raman scattering [93Miz].

KH_2PO_4				KD_2PO_4			
	Neutron		Raman		Neutron		Raman
Mode	E [meV]	Γ [meV]	E [meV]	Mode	E [meV]	Γ [meV]	E [meV]
H				D			
	161(3)	7.3	161.9		106(2)	4.9	119.5
	126(3)	7.7	125.7		87(2)	4.8	88.3
PO_4				PO_4			
ν_3	145(3)	9.4	142.3	ν_3	144(3)	14.8	147.5
	–	–	134.2		–	–	136.9
	–	–	118.8		–	–	122.0
	116(2)	13.7	113.6		115(2)	9.3	116.6
ν_1	101(2)	3.8	113.6	ν_1	99(2)	2.3	108.4
ν_4	87(2)	6.4	72.9	ν_4	78(2)	5.3	69.2
	70(1)	3.1	67.9		66(1)	2.6	66.0
	63(1)	4.0	64.7		62(1)	3.4	62.7
	57(1)	5.0	58.3		57(1)	3.9	57.8
ν_2	52(1)	2.2	49.6	ν_2	49(1)	2.4	47.4
	44(1)	2.9	43.4		44.(1)	2.6	44.6