Table 33A-3-001. CsH_2PO_4 (CDP). Lattice parameters and unit cell volume at several temperatures [78Ras].

Cell parameters	298 K	160 K	144 K	70 K	6.4 K
a [Å]	7.917(2)	7.903(2)	7.904(4)	7.899(6)	7.886(3)
b [Å]	6.365(2)	6.328(2)	6.316(3)	6.289(7)	6.259(4)
c [Å]	4.876(1)	4.892(2)	4.895(3)	4.892(4)	4.914(2)
β [deg]	107.84(2)	108.16(2)	108.23(4)	108.32(5)	108.55(3)
V [Å^3]	233.9(2)	232.9(3)	232.1(4)	230.7(7)	229.9(4)

Table 33A-3-002. CsH_2PO_4 (CDP). Fractional coordinates and anisotropic temperature parameters for nonhydrogen atoms at RT [80Mat]. Anisotropic temperature parameter U_{ij} [$\cdot 10^{-2}$ Å^2] is defined by Eq. (d) in Introduction. For hydrogen atoms isotropic temperature parameters are given.

	x	y	z	U_{11}, B	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cs	0.26569(6)	0.25	0.0354(1)	3.09(2)	2.60(2)	2.34(2)	0.0	0.64(2)	0.0
P	0.2370(2)	0.75	0.5293(3)	1.91(7)	2.41(8)	1.20(7)	0.0	0.75(6)	0.0
O(1)	0.3898(6)	0.75	0.3874(10)	2.1(2)	3.7(3)	1.5(2)	0.0	0.9(2)	0.0
O(2)	0.3222(5)	0.75	0.8447(11)	4.3(3)	6.1(4)	1.3(2)	0.0	1.3(2)	0.0
O(3)	0.1266(5)	0.5540(7)	0.4178(9)	4.3(2)	3.6(2)	4.2(2)	−1.2(2)	2.4(2)	−1.6(2)
H(1)	0.348(13)	0.75	0.195(24)	2.1(28)					
H(2)	0.0	0.5	0.5	5.5(41)					

Table 33A-3-003. CsH_2PO_4 (CDP). Fractional coordinates and anisotropic temperature parameters at 83 K by neutron diffraction experiment [80Iwa]. Anisotropic temperature parameter b_{ij} is defined by Eq. (b) in Introduction. Values of b_{ij} multiplied by 10^4 are shown.

	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
Cs	0.2635(3)	0.25	0.0275(4)	28(3)	28(5)	57(7)	−12(22)	19(20)	11(7)
P	0.2403(3)	0.7396(9)	0.5300(4)	18(3)	14(6)	35(7)	−18(23)	−7(19)	10(7)
O(1)	0.3965(3)	0.7526(9)	0.3947(4)	27(3)	44(6)	47(6)	−16(20)	−31(18)	24(7)
O(2)	0.3252(3)	0.7431(9)	0.8496(4)	47(3)	70(6)	33(6)	18(21)	18(20)	25(7)
O(3)	0.1237(4)	0.5519(5)	0.4155(5)	44(4)	30(6)	103(8)	−42(13)	−32(12)	33(9)
O(4)	0.1316(4)	0.9534(5)	0.4155(5)	43(4)	21(6)	126(9)	−2(14)	13(13)	62(9)
H(1)	0.3597(6)	0.7432(16)	0.1796(7)	83(6)	73(9)	127(12)	27(44)	4(35)	56(14)
H(2)	0.9738(6)	0.4899(14)	0.5152(9)	56(8)	100(12)	153(14)	−32(26)	26(22)	80(17)

Table 33A-3-004. CsD_2PO_4 (DCDP). Fractional coordinates and isotropic temperature parameters at 283 K [83Ito]. The prime stands for the split atom. Deuteration rate: 0.97.

Atom	x	y	z	$\overline{u^2}$ [$\cdot 10^{-2}$ Å^2]
Cs	0.26471(2)	0.25	0.03156(3)	2.492(3)
P′	0.23901(8)	0.763(1)	0.5288(1)	1.62(7)
O(1)′	0.3942(2)	0.753(2)	0.3894(4)	2.53(4)
O(2)′	0.3237(4)	0.758(6)	0.8463(5)	4.0(2)
O(3)′	0.136(2)	0.546(2)	0.433(3)	4.9(2)
O(4)′	0.124(1)	0.942(2)	0.407(2)	3.3(1)
D(1)	0.361(9)	0.75	0.22(2)	1.4(11)
D(2)	0.0	0.5	0.5	9.8(80)

Table 33A-3-005. CsD_2PO_4 (DCDP). Fractional coordinates and isotropic temperature parameters at 233 K [83Ito]. Deuteration rate: 0.97.

Atom	x	y	z	$\overline{u^2}$ [$\cdot 10^{-2}$ Å^2]
Cs	0.26422(2)	0.25	0.02982(3)	2.008(3)
P	0.23958(7)	0.7647(2)	0.5290(1)	1.29(1)
O(1)	0.3946(2)	0.758(1)	0.3903(3)	2.02(4)
O(2)	0.3241(3)	0.755(2)	0.8465(4)	3.23(5)
O(3)	0.1375(9)	0.5499(7)	0.425(2)	3.9(1)
O(4)	0.1211(7)	0.9465(7)	0.410(1)	2.57(6)
D(1)	0.365(6)	0.77(2)	0.20(1)	0.2(10)
D(2)	−0.059(8)	0.49(1)	0.48(1)	0.5(11)

Table 33A-3-006. CsH_2PO_4 (CDP). Fractional coordinates and anisotropic temperature parameters in phase VII [85Sch]. $p = 3.6 \cdot 10^8$ Pa, $T = 100.7(5)$ K. Anisotropic temperature parameter U_{ij} [Å^2] is defined by Eq. (d) in Introduction.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cs(1)	0.1312(3)	0.25	0.2385(8)	0.024(2)	0.010(2)	0.009(2)	0.002(3)	0.009(2)	0.0002(24)
P(1)	0.1206(3)	0.7400(10)	0.7137(9)	0.020(2)	0.009(2)	0.008(2)	−0.006(2)	0.006(2)	−0.005(2)
O(11)	0.1626(3)	0.7470(10)	0.4772(8)	0.026(2)	0.023(2)	0.009(2)	0.0001(26)	0.012(2)	0.005(2)
O(12)	0.1992(2)	0.7535(9)	1.0063(9)	0.020(2)	0.019(2)	0.010(2)	−0.005(3)	0.008(2)	−0.008(3)
O(13)	0.0630(4)	0.5494(7)	0.7104(10)	0.028(3)	0.001(2)	0.016(3)	−0.005(2)	0.0003(20)	−0.001(2)
O(14)	0.0658(4)	0.9514(8)	0.7183(11)	0.025(3)	0.023(3)	0.011(3)	−0.0003(22)	0.013(2)	−0.007(2)
H(121)	0.1814(5)	0.7456(15)	1.1864(16)	0.034(4)	0.031(4)	0.015(4)	−0.009(4)	0.013(3)	0.006(4)
H(143)	0.9874(6)	0.4885(14)	0.4631(18)	0.027(5)	0.017(4)	0.021(5)	−0.010(4)	0.009(4)	−0.008(3)
Cs(2)	0.6311(2)	0.2538(8)	0.2381(8)	0.012(2)	0.012(2)	0.014(2)	0.002(2)	0.010(2)	−0.0003(25)
P(2)	0.6201(3)	0.7656(10)	0.7126(8)	0.015(2)	0.009(2)	0.009(2)	−0.006(2)	0.008(2)	−0.0001(25)
O(21)	0.6624(3)	0.7606(9)	0.4774(8)	0.020(2)	0.020(2)	0.012(2)	−0.0003(24)	0.012(2)	0.007(2)
O(22)	0.6995(2)	0.7596(9)	1.0068(9)	0.010(2)	0.015(2)	0.012(2)	−0.003(2)	0.007(2)	−0.003(3)
O(23)	0.5660(4)	0.5542(7)	0.7170(11)	0.023(3)	0.004(2)	0.016(3)	−0.006(2)	−0.0004(21)	−0.002(2)
O(24)	0.5614(3)	0.9591(8)	0.7099(10)	0.014(2)	0.025(3)	0.012(2)	0.002(2)	0.012(2)	−0.003(2)
H(221)	0.6808(4)	0.7587(15)	1.1851(16)	0.021(4)	0.028(4)	0.018(4)	−0.004(4)	0.005(3)	0.004(4)
H(234)	0.5109(6)	0.5179(16)	0.5345(21)	0.012(4)	0.029(4)	0.037(5)	0.014(4)	0.010(4)	0.009(4)

Table 33A-3-007. CsH_2PO_4 (CDP). Fractional coordinates and isotropic temperature parameter *B* at RT [76Ues]. *B* is defined by Eq. (e) in Introduction.

Atom	Wyckoff notation	*x*	*y*	*z*	*B* [Å²]
Cs	e	0.2659 (3)	0.2500	0.0357 (5)	1.04 (3)
P	e	0.2342 (7)	0.7500	0.5308 (12)	0.74 (14)
O1	e	0.3935 (22)	0.7500	0.3900 (35)	1.33 (23)
O2	e	0.3256 (30)	0.7500	0.8413 (45)	3.86 (35)
O3	f	0.1232 (22)	0.5524 (29)	0.4155 (36)	2.99 (28)

Table 33A-3-008. CsH_2PO_4 (CDP). Fractional coodinates in a pseudo-orthorhombic cell at RT [78Nel].

Atom	Site symmetry	*x*	*y*	*z*
Cs	m	0.0965 (7)	0.25	0.1331 (2)
P	m	0.5899 (6)	0.75	0.1187 (2)
O1	m	0.8091 (6)	0.75	0.1955 (2)
O2	m	0.3152 (6)	0.75	0.1613 (2)
O3	l	0.6454 (6)	0.5530 (5)	0.0633 (2)
H1	m	0.495 (1)	0.25	0.3226 (3)
H2	l	0.973 (5)	0.500 (6)	0.487 (1)

Table 33A-3-009. $CsH_{2(1-x)}D_{2x}PO_4$. Fractional coordinates and isotropic thermal parameter [94Iwa]. Isotropic temperature parameter *B* [Å²] is defined by Eq. (e) in Introduction.

1) $x = 0.0$

	x	*y*	*z*	*B*
Cs	0.2632(3)	0.25	0.0269(5)	1.48(3)
P	0.2405(3)	0.7362(7)	0.5295(5)	1.28(3)
O(1)	0.3960(3)	0.7489(7)	0.3945(5)	1.52(3)
O(2)	0.3254(3)	0.7438(8)	0.8499(5)	1.77(3)
O(3)	0.1206(4)	0.5486(5)	0.4111(6)	1.64(3)
O(4)	0.1350(4)	0.9506(5)	0.4206(6)	1.80(4)
H(1)	0.9731(7)	0.4873(11)	0.5129(13)	2.43(8)
H(2)	0.3592(6)	0.7423(16)	0.1795(10)	2.39(6)

2) $x = 0.36$

	x	*y*	*z*	*B*
Cs	0.2628(3)	0.25	0.0265(5)	1.68(4)
P	0.2405(3)	0.7360(7)	0.5295(5)	1.49(4)
O(1)	0.3970(3)	0.7473(7)	0.3940(5)	1.66(3)
O(2)	0.3254(3)	0.7444(8)	0.8501(5)	1.87(4)
O(3)	0.1219(4)	0.5479(5)	0.4124(7)	1.91(4)
O(4)	0.1353(4)	0.9505(5)	0.4198(7)	1.97(5)
H(1)	0.9721(–)	0.4855(–)	0.5123(–)	2.9(–)
H(2)	0.3599(–)	0.7426(–)	0.1799(–)	2.4(–)

Table 33A-3-009 (continued).

3) $x = 0.57$

	x	*y*	*z*	*B*
Cs	0.2630(3)	0.25	0.0264(8)	1.64(4)
P	0.2409(3)	0.7356(8)	0.5291(8)	1.49(4)
O(1)	0.3970(3)	0.7469(8)	0.3955(8)	1.75(3)
O(2)	0.3261(4)	0.7423(9)	0.8513(8)	2.07(4)
O(3)	0.1218(4)	0.5481(5)	0.4123(10)	1.82(4)
O(4)	0.1369(4)	0.9497(5)	0.4211(10)	1.86(4)
H(1)	0.9684(13)	0.4842(18)	0.5056(33)	2.7(2)
H(2)	0.3601(9)	0.7441(22)	0.1819(20)	2.19(9)

4) $x = 0.79$

	x	*y*	*z*	*B*
Cs	0.2625(3)	0.25	0.0248(8)	1.38(3)
P	0.2414(4)	0.7353(7)	0.5296(8)	1.25(4)
O(1)	0.3977(3)	0.7476(8)	0.3961(7)	1.53(3)
O(2)	0.3263(4)	0.7429(8)	0.8511(8)	1.74(4)
O(3)	0.1210(4)	0.5477(5)	0.4124(9)	1.58(4)
O(4)	0.1371(4)	0.9501(5)	0.4212(9)	1.59(4)
H(1)	0.9698(5)	0.4839(9)	0.5090(14)	2.09(7)
H(2)	0.3609(5)	0.7423(12)	0.1844(11)	2.30(6)

5) $x = 1.0$

	x	*y*	*z*	*B*
Cs	0.2621(3)	0.25	0.0239(5)	1.57(3)
P	0.2415(3)	0.7370(8)	0.5296(6)	1.48(3)
O(1)	0.3974(3)	0.7482(7)	0.3952(5)	1.58(3)
O(2)	0.3263(3)	0.7427(8)	0.8492(6)	1.85(3)
O(3)	0.1221(4)	0.5477(5)	0.4120(6)	1.75(4)
O(4)	0.1368(4)	0.9497(5)	0.4188(6)	1.82(4)
H(1)	0.9710(3)	0.4836(6)	0.5116(7)	2.21(4)
H(2)	0.3605(3)	0.7428(7)	0.1803(5)	2.20(3)

Table 33A-3-010. CsH_2PO_4 (CDP). Root-mean-square displacements of atoms (r.m.s.) and their principal directions at RT [80Mat]. ϕ_a, ϕ_b, ϕ_c: angles between the principal directions 1, 2, 3 and the crystallographic *a*, *b*, *c* axes.

		r.m.s.	ϕ_a	ϕ_b	ϕ_c
Cs	1	0.18 Å	5°	90°	113°
	2	0.16	90	0	90
	3	0.15	85	90	23
P	1	0.16	90	0	90
	2	0.14	152	90	101
	3	0.10	118	90	11
O(1)	1	0.19	90	0	90
	2	0.15	143	90	110
	3	0.11	53	90	160
O(2)	1	0.25	90	0	90
	2	0.21	162	90	90
	3	0.10	108	90	0
O(3)	1	0.25	63	124	58
	2	0.17	150	116	62
	3	0.15	101	45	45
H(1)		0.14			
H(2)		0.23			

Table 33A-3-011. CsH_2PO_4 (CDP). Interatomic distances and bond angles of phosphate group and hydrogen bond at RT [80Mat]. For numbering of the atoms, see Fig. 33A-3-009.

Phosphate group			
P–O(1)	1.565(6) Å	O(1)–P–O(2)	107.0(3)°
P–O(2)	1.481(5)	O(1)–P–O(3)	106.1(2)
P–O(3)	1.529(4)	O(1)–P–O(4)	106.1(2)
P–O(4)	1.529(4)	O(2)–P–O(3)	113.6(2)
		O(2)–P–O(4)	113.6(2)
		O(3)–P–O(4)	109.9(2)
Hydrogen bond			
O(1)–O(2^{i})	2.537(7) Å	O(1)–H(1)–O(2^{i})	166(11)°
O(1)–H(1)	0.9(1)		
H(1)···O(2^{i})	1.7(1)		
O(3)–O(3^{ii})	2.472(7)		

Table 33A-3-012. CsH_2PO_4 (CDP). Interatomic distances and angles related with O–H···O bonds at RT [78Nel]. H1 is a special position on the mirror plane. H2 is a special position at the center of inversion ($\bar{1}$). O3 is a general position. O3 and O3′ are related by the center of inversion at the H2 site (0, 1/2, 1/2); H2 and H2′ are symmetrically displaced from (0, 1/2, 1/2) along the O3–O3′ line.

O1–H1···O2		O3–H2–H2′–O3′	
Distances [Å]:			
O1–H1	0.995 (7)	O3–H2	1.00 (2)
H1···O2	1.530 (7)	H2···O3′	1.46 (2)
O1···O2	2.521 (7)	O3···O3′	2.46 (1)
		H2–H2′	0.48 (4)
Angles [°]:			
O1–H1···O2	173.2 (5)	O3–H2···O3′	174 (4)

Table 33A-3-013. CsH_2PO_4 (CDP). Ultrasonic velocities at RT [85Pra]. f = 10 MHz. $\boldsymbol{x} \parallel \boldsymbol{a}^*$, $\boldsymbol{y} \parallel \boldsymbol{b}$, $\boldsymbol{z} \parallel \boldsymbol{c}$. PT: pure transverse. PL: pure longitudinal. SPT: semi-pure transverse. SPL: semi-pure longitudinal. QT: quasi-transverse. QL: quasi-longitudinal.

No.	Direction of wave propagation	Approximate wave displacement direction	Velocity [$\cdot 10^3$ m s^{-1}]	Type
1	100	100	3.047(5)	SPL
2	100	010	1.688(20)	PT
3	100	001	1.133(10)	SPT
4	010	010	2.878(20)	PL
5	010	100	1.788(20)	PT
6	010	001	1.416(2)	PT
7	001	001	4.540(10)	SPL
8	001	010	1.586(15)	PT
9	001	100	1.153(3)	SPT
10	0.520, 0, −0.854	0.520, 0, −0.854	3.847(6)	SPL
11	0.520, 0, −0.854	010	1.796(4)	PT
12	0.520, 0, −0.854	0.854, 0, 0.520	0.7605(6)	SPT
13	110	110	2.982(6)	QL
14	110	001	1.683(3)	QT
15	110	$\bar{1}10$	1.307(13)	QT
16	011	011	3.622(80)	QL
17	011	$0\bar{1}1$	1.980(8)	QT
18	011	100	1.409(7)	QT
19	0.252, 0.588, −0.769	0.252, 0.588, −0.769	3.686(80)	QL
20	0.252, 0.588, −0.769	Trans 1	2.014(10)	QT
21	0.252, 0.588, −0.769	Trans 2	1.219(9)	QT
22	0.698, 0, −0.716	0.698, 0, −0.716	3.217(130)	SPL
23	0.698, 0, −0.716	010	1.796(4)	PT
24	0.698, 0, −0.716	0.716, 0, 0.698	Unknown	SPT
25	0.925, 0, 0.395	0.925, 0, 0.395	3.151(4)	SPL
26	0.925, 0, 0.395	010	1.520(4)	PT
27	0.925, 0, 0.395	0.395, 0, −0.925	0.83(3)	SPT

Table 33A-3-014. CsD_2PO_4 (DCDP). e^2qQ/h, η and μ at deuteron sites [80Top]. μ_a, μ_b, μ_c are direction cosines of the principal axes of the deuteron EFG tensor with respect to the crystallographic a^*, b, c axes, respectively. ϕ_{ij}: component of EFG tensor; η: asymmetry parameter.

			ϕ_{zz}	ϕ_{yy}	ϕ_{xx}
$T = 23$ °C ($T > \Theta_f$)					
Site					
D(1)	$e^2qQ/h = 167$ kHz	$\mu_a =$	0.958	0.091	0.272
	$\eta = 0.04$	$\mu_b =$	−0.022	0.969	−0.246
		$\mu_c =$	−0.286	0.229	0.930
D(2)	$e^2qQ/h = 121$ kHz	$\mu_a =$	0.578	−0.310	0.754
	$\eta = 0.05$	$\mu_b =$	−0.292	0.788	0.548
		$\mu_c =$	0.762	0.534	−0.361
D(2)′	$e^2qQ/h = 121$ kHz	$\mu_a =$	0.586	0.705	−0.157
	$\eta = 0.05$	$\mu_b =$	0.261	−0.004	0.965
		$\mu_c =$	0.767	−0.606	−0.210
$T = -21$ °C ($T < \Theta_f$)					
D(1)	$e^2qQ/h = 170$ kHz	$\mu_a =$	0.958	0.022	0.284
	$\eta = 0.06$	$\mu_b =$	−0.038	0.998	0.054
		$\mu_c =$	−0.282	−0.059	0.957
D(1)′	$e^2qQ/h = 164$ kHz	$\mu_a =$	0.958	0.157	0.241
	$\eta = 0.03$	$\mu_b =$	−0.009	0.856	−0.539
		$\mu_c =$	−0.288	0.492	0.807
D(2)	$e^2qQ/h = 121$ kHz	$\mu_a =$	0.578	−0.310	0.754
	$\eta = 0.05$	$\mu_b =$	−0.292	0.788	0.548
		$\mu_c =$	0.762	0.534	−0.361
D(2)′	$e^2qQ/h = 121$ kHz	$\mu_a =$	0.586	0.705	−0.157
	$\eta = 0.05$	$\mu_b =$	0.261	−0.004	0.965
		$\mu_c =$	0.767	−0.606	−0.210

Table 33A-3-015. CsH_2PO_4 (CDP). Spin Hamiltonian parameters and direction cosines (with respect to a^*, b, c frame) for Cu^{2+} ion [85Wap].

Spin Hamiltonian parameters	Direction cosines of Z principal axis*		
	l	m	n
$g_{\parallel} = 2.2575$	0.0292	0.1736	0.9698
$g_{\perp} = 2.1866$			
$A_{\parallel} = 0.32\ m^{-1}$			
$A_{\perp} = 0.28\ m^{-1}$			

* with respect to the a^*, b, c axes.

Table 33A-3-016. CsH_2PO_4 (CDP). Principal values and direction cosines of D tensor for Cr^{3+} [80Tak]. Direction cosines refer to the (a^*, b, c) frame.

a) $T = 164$ K

	Principal values [$\cdot 10^2$ A m^{-1}]	Direction cosine		
		l	m	n
D_X	39(8)	0.224	−0.313	−0.923
D_Y	−1569(8)	−0.665	0.643	−0.380
D_Z	1531(8)	0.712	0.699	−0.064

b) $T = 116$ K

	Principal values [$\cdot 10^2$ A m^{-1}]	Direction cosine		
		l	m	n
Cr^{3+}(I)				
D_X	33(8)	0.226	−0.312	−0.923
D_Y	−1574(8)	−0.665	0.644	−0.380
D_Z	1541(8)	0.712	0.699	−0.062
Cr^{3+}(II)				
D_X	181(8)	0.134	−0.506	−0.854
D_Y	−1476(8)	−0.678	0.581	−0.449
D_Z	1295(8)	0.723	0.639	−0.264

Table 33A-3-017. CsH_2PO_4 (CDP). g-tensor values for $(CrO_4)^{3-}$ ESR [84Wap].

	Direction cosine *)		
	l	m	n
$T = 300$ K			
$g_{\parallel} = 1.9539$	0.7071	0.7071	0
$g_{\perp} = 1.9789$			
$T = 160$ K			
$g_{zz} = 1.9452$	0	±0.7071	±0.7071
$g_{xx} = 1.9764$	0	∓0.7071	±0.7071
$g_{yy} = 1.9848$	1	0	0

* with respect to the a^*, b, c axes.

Table 33A-3-018. CsH_2PO_4 (CDP). Principal values and direction cosines of A tensor for $(AsO_3)^{2-}$ [80Tak]. Direction cosines refer to the (a^*, b, c) frame.

	Principal values [$\cdot 10^2$ A m^{-1}]	Direction cosine		
		l	m	n
$T = 175$ K				
AsO_3^{2-}(A)				
A_X	451(6)	0.707	0.0	0.707
A_Y	467(6)	0.0	1.0	0.0
A_Z	583(6)	0.707	0.0	−0.707
AsO_3^{2-}(B)				
A_X	453(6)	−0.799	∓0.573	0.185
A_Y	446(6)	0.174	±0.073	0.982
A_Z	577(6)	−0.576	∓0.816	−0.041
$T = 105$ K				
AsO_3^{2-}(A)				
A_X	459(6)	0.707	0.0	0.707
A_Y	477(6)	±0.059	0.995	∓0.059
A_Z	589(6)	0.705	±0.084	−0.705