Table 33A-5-001. $NH_4H_2PO_4$ (ADP), $ND_4D_2PO_4$ (DADP). Unit cell parameters in phase I [87Fuk1].

		$NH_4H_2PO_4$				$ND_4D_2PO_4$			
	T [K]	152	195	245	296	243	283	323	364
Unit cell parameters [Å]	$a=b$	7.473(1)	7.483(1)	7.493(1)	7.505(1)	7.513(1)	7.522(1)	7.532(1)	7.542(1)
	c	7.551(2)	7.554(1)	7.558(1)	7.558(1)	7.542(1)	7.546(1)	7.546(1)	7.545(1)

Table 33A-5-002. $ND_4D_2PO_4$ (DADP). Unit cell parameters in phase II [88Fuk2].

T [K]		140	171	195	235
Unit cell parameters [Å]	a	7.526(1)	7.530(1)	7.533(1)	7.538(1)
	b	7.551(1)	7.553(1)	7.557(1)	7.558(1)
	c	7.464(1)	7.469(1)	7.475(1)	7.483(1)

Table 33A-5-003. $NH_4H_2PO_4$ (ADP), $NH_4H_2AsO_4$ (ADA). Fractional coordinates and temperature parameters at RT [73Kha]. b_{ij} is defined by Eq. (b) in Introduction. b_{ij} is in the unit of 10^{-4}. Isotropic temperature parameters for the H atoms defined in Eq. (e) of Introduction are listed under b_{11}. See Fig. 33A-5-004 for H(n) and H(o).

	Site symmetry	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
$NH_4H_2PO_4$ (ADP)										
P	$\bar{4}$	0	0	0	55(1)	55(1)	84(1)	0	0	0
N	$\bar{4}$	0	0	1/2	110(2)	110(2)	88(3)	0	0	0
O	1	0.0843(1)	0.1466(1)	0.1151(1)	75(2)	83(2)	118(2)	13(1)	–22(2)	–37(2)
H(N)	1	–0.002(5)	0.089(3)	0.563(2)	2.8(5)Å^2					
H(O)	2	1/4	0.150(6)	1/8	5(1) Å^2					
$NH_4H_2AsO_4$ (ADA)										
As	$\bar{4}$	0	0	0	57(1)	57(1)	89(1)	0	0	0
N	$\bar{4}$	0	0	1/2	112(2)	112(2)	89(3)	0	0	0
O	1	0.0869(2)	0.1578(2)	0.1233(2)	78(2)	88(2)	145(2)	19(1)	–28(2)	–48(2)
H(N)	1	0.014(5)	0.120(3)	0.567(3)	2.4(6) Å^2					
H(O)	2	1/4	0.199(9)	1/8	4.6(2) Å^2					

Table 33A-5-004. $NH_4H_2PO_4$ (ADP), $ND_4D_2PO_4$ (DADP). Fractional coordinates and temperature parameters in phase I [87Fuk1]. U_{ij} [$\cdot 10^{-4}$ Å^2] is defined by Eq. (d) in Introduction. See Fig. 33A-5-004 for H(n) and H(o).

Atom	T [K]	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
$NH_4H_2PO_4$										
P	152	0	0	0	77(2)	77(2)	133(2)	0	0	0
	195	0	0	0	97(2)	97(2)	161(2)	0	0	0
	245	0	0	0	120(3)	120(3)	192(3)	0	0	0
	296	0	0	0	147(3)	147(3)	230(3)	0	0	0
N	152	0	0	0.5	176(9)	176(9)	118(6)	0	0	0
	195	0	0	0.5	211(11)	211(11)	144(8)	0	0	0
	245	0	0	0.5	253(14)	253(14)	181(9)	0	0	0
	296	0	0	0.5	308(18)	308(18)	212(11)	0	0	0
O	152	0.0843(1)	0.1479(1)	0.1153(1)	108(3)	120(3)	172(3)	18(2)	−32(3)	−57(3)
	195	0.0844(2)	0.1476(2)	0.1153(2)	134(3)	148(3)	213(4)	22(3)	−41(4)	−72(4)
	245	0.0844(2)	0.1471(2)	0.1154(2)	165(4)	182(4)	261(5)	29(4)	−51(4)	−86(5)
	296	0.0844(2)	0.1466(2)	0.1154(3)	201(5)	220(5)	314(7)	37(4)	−63(5)	−102(6)
H(n)	152	0.001(6)	0.091(4)	0.568(3)	2.9(6)					
	195	−0.008(7)	0.095(5)	0.567(3)	3.6(8)					
	245	−0.012(7)	0.087(5)	0.566(3)	3.5(9)					
	296	−0.016(8)	0.090(5)	0.567(4)	5(1)					
H(o)	152	0.25	0.168(8)	0.125	6(1)					
	195	0.25	0.16(1)	0.125	7(2)					
	245	0.25	0.16(1)	0.125	7(2)					
	296	0.25	0.16(1)	0.125	8(2)					
$ND_4D_2PO_4$										
P	243	0	0	0	123(3)	123(3)	206(3)	0	0	0
	283	0	0	0	136(4)	136(4)	222(4)	0	0	0
	323	0	0	0	154(4)	154(4)	241(4)	0	0	0
	364	0	0	0	164(4)	164(4)	252(5)	0	0	0
N	243	0	0	0.5	276(17)	276(17)	176(10)	0	0	0
	283	0	0	0.5	314(21)	314(21)	200(13)	0	0	0
	323	0	0	0.5	347(22)	347(22)	232(13)	0	0	0
	364	0	0	0.5	380(30)	380(30)	250(18)	0	0	0
O	243	0.0832(2)	0.1473(2)	0.1154(2)	170(5)	188(5)	273(6)	32(4)	−54(5)	−91(5)
	283	0.0832(2)	0.1468(2)	0.1154(3)	192(6)	210(6)	300(7)	38(5)	−59(6)	−103(7)
	323	0.0833(2)	0.1464(2)	0.1154(3)	219(6)	238(6)	331(7)	45(5)	−67(6)	−111(7)
	364	0.0832(3)	0.1459(3)	0.1155(4)	238(8)	254(8)	352(10)	50(7)	−70(9)	−119(9)
D(n)	243	0.015(7)	0.093(5)	0.564(4)	2.5(7)					
	283	0.022(7)	0.097(6)	0.564(4)	2.3(8)					
	323	0.017(7)	0.098(6)	0.563(4)	2.8(8)					
	364	0.017(8)	0.102(6)	0.562(4)	2.3(8)					
D(o)	243	0.25	0.15(1)	0.125	6(2)					
	283	0.25	0.15(1)	0.125	4(2)					
	323	0.25	0.15(1)	0.125	4(1)					
	364	0.25	0.15(1)	0.125	3(1)					

Table 33A-5-005. $NH_4H_2PO_4$ (ADP). Fractional coordinates and temperature parameters at 143 K in phase II [87Fuk2]. U_{ij} [$\cdot 10^{-4}$ 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}
P	0.0000(0)	0.0019(0)	0.0004(0)	71(1)	73(1)	95(1)	−1(1)	−4(1)	2(1)
N	0.0110(1)	−0.0163(1)	0.5016(1)	132(3)	116(3)	116(2)	14(3)	1(3)	−6(2)
O(1)	0.0820(1)	0.1443(1)	0.1192(1)	111(3)	114(3)	165(3)	19(2)	−38(2)	−55(3)
O(2)	−0.0853(1)	−0.1502(1)	0.1145(1)	100(2)	122(3)	155(3)	17(2)	34(2)	53(2)
O(3)	−0.1372(1)	0.0773(1)	−0.1280(1)	108(2)	109(2)	131(2)	−13(2)	−41(2)	27(2)
O(4)	0.1571(1)	−0.0900(1)	−0.1026(1)	100(2)	100(2)	163(3)	−11(2)	39(2)	−26(2)
H(n1)	0.012(3)	0.074(3)	0.587(3)	1.7(4)					
H(n2)	0.000(4)	−0.112(4)	0.547(4)	3.1(5)					
H(n3)	−0.068(3)	0.004(3)	0.421(3)	2.5(5)					
H(n4)	0.113(3)	−0.013(3)	0.453(3)	2.0(5)					
H(o1)	−0.211(4)	−0.152(4)	0.122(4)	3.4(6)					
H(o2)	0.154(4)	−0.202(3)	−0.108(3)	3.1(6)					

Table 33A-5-006. $ND_4D_2PO_4$ (DADP). Fractional coordinates and temperature parameters in phase II [88Fuk2]. Parameter: T. U_{ij} [$\cdot 10^{-4}$ Å^2] is defined by Eq. (d) in Introduction.

T[K]	Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
235	P	−0.0012(1)	0.0019(1)	0.0005(1)	112(1)	114(1)	148(1)	4(2)	−5(2)	1(1)
	N	0.0129(3)	−0.0184(2)	0.5019(3)	204(7)	162(6)	174(5)	32(6)	11(6)	−8(5)
	O(1)	0.0799(2)	0.1425(2)	0.1206(3)	193(6)	180(6)	264(7)	48(5)	−66(6)	−93(6)
	O(2)	−0.0848(2)	−0.1503(2)	0.1140(3)	154(5)	205(6)	251(7)	33(5)	64(6)	95(6)
	O(3)	−0.1354(2)	0.0753(2)	−0.1300(2)	172(5)	171(5)	190(5)	−15(5)	−56(5)	36(5)
	O(4)	0.1567(2)	−0.0894(2)	−0.1010(2)	143(5)	153(5)	249(7)	−19(4)	59(5)	−48(5)
	D(n1)	0.014(6)	0.085(5)	0.596(5)	2.7(8)					
	D(n2)	0.015(7)	−0.089(6)	0,538(6)	4(1)					
	D(n3)	−0.069(5)	0.023(6)	0.397(6)	4(1)					
	D(n4)	0.102(6)	0.000(6)	0.454(5)	2.8(8)					
	D(o1)	−0.190(5)	−0.155(5)	0.125(5)	2.3(7)					
	D(o2)	0.148(4)	−0.178(4)	−0.098(4)	1.3(6)					
195	P	−0.0010(1)	0.0019(1)	0.0005(1)	94(1)	97(1)	125(1)	2(2)	−2(2)	0(1)
	N	0.0130(3)	−0.0188(2)	0.5019(2)	169(6)	138(5)	152(5)	33(5)	9(5)	−5(4)
	O(1)	0.0801(2)	0.1424(2)	0.1205(2)	165(5)	158(5)	229(7)	38(5)	−53(5)	−76(5)
	O(2)	−0.0845(2)	−0.1506(2)	0.1143(2)	136(5)	179(6)	211(6)	33(4)	57(5)	87(5)
	O(3)	−0.1352(2)	0.0751(2)	−0.1305(2)	152(5)	150(5)	158(5)	−11(4)	−51(4)	30(4)
	O(4)	0.1575(2)	−0.0897(2)	−0.1010(2)	124(4)	128(5)	216(6)	−18(4)	48(5)	−43(5)
	D(n1)	0.016(5)	0.086(5)	0.597(5)	2.0(7)					
	D(n2)	0.012(7)	−0.092(7)	0.542(7)	5(1)					
	D(n3)	−0.071(6)	0.023(6)	0.392(6)	4(1)					
	D(n4)	0.100(6)	−0.004(6)	0.456(5)	2.4(8)					
	D(o1)	−0.195(5)	−0.156(5)	0.125(5)	2.4(8)					
	D(o2)	0.148(4)	−0.179(4)	−0.100(4)	0.8(5)					
171	P	−0.0009(1)	0.0019(1)	0.0005(1)	84(1)	87(1)	113(1)	2(2)	−6(1)	1(1)
	N	0.0132(2)	−0.0188(2)	0.5017(2)	155(5)	117(5)	136(5)	32(5)	7(5)	−3(4)
	O(1)	0.0801(2)	0.1427(2)	0.1206(2)	160(5)	147(5)	208(6)	35(5)	−52(5)	−72(5)
	O(2)	−0.0845(2)	−0.1508(2)	0.1142(2)	116(4)	166(5)	191(6)	32(4)	54(5)	79(5)
	O(3)	−0.1352(2)	0.0751(2)	−0.1304(2)	138(4)	139(5)	142(5)	−7(4)	−43(4)	27(4)
	O(4)	0.1576(2)	−0.0897(2)	−0.1010(2)	106(4)	118(4)	192(5)	−14(4)	41(4)	−41(4)
	D(n1)	0.018(6)	0.089(5)	0.597(6)	2.4(9)					
	D(n2)	0.011(7)	−0.093(7)	0.544(7)	4(1)					
	D(n3)	−0.069(6)	0.023(6)	0.394(7)	3(1)					
	D(n4)	0.104(5)	−0.002(6)	0.456(5)	2.0(8)					
	D(o1)	−0.200(5)	−0.156(5)	0.124(5)	2.1(8)					
	D(o2)	0.151(5)	−0.183(5)	−0.099(5)	1.2(6)					
140	P	−0.0007(1)	0.0019(1)	0.0006(1)	70(1)	73(1)	93(1)	0(1)	−3(1)	1(1)
	N	0.0134(2)	−0.0188(2)	0.5020(2)	129(5)	102(4)	119(4)	30(4)	4(5)	−6(4)
	O(1)	0.0803(2)	0.1428(2)	0.1206(2)	131(5)	125(5)	185(6)	25(4)	−47(5)	−65(5)
	O(2)	−0.0844(2)	−0.1510(2)	0.1143(2)	104(4)	141(5)	166(5)	27(4)	48(4)	69(4)
	O(3)	−0.1354(2)	0.0751(2)	−0.1304(2)	116(4)	114(4)	118(4)	−3(4)	−36(4)	24(4)
	O(4)	0.1508(2)	−0.0899(2)	−0.1009(2)	90(4)	106(4)	161(5)	−14(3)	33(4)	−33(4)
	D(n1)	0.020(6)	0.086(5)	0.595(6)	2.1(8)					
	D(n2)	0.008(8)	−0.093(8)	0.542(7)	5(1)					
	D(n3)	−0.074(6)	0.018(6)	0.397(6)	3(1)					
	D(n4)	0.106(6)	−0.007(6)	0.458(5)	2.2(8)					
	D(o1)	−0.199(6)	−0.158(6)	0.125(6)	2.3(8)					
	D(o2)	0.148(5)	−0.185(5)	−0.098(5)	1.5(7)					

Table 33A-5-007. $NH_4H_2PO_4$ (ADP), $ND_4D_2PO_4$ (DADP). Fractional coordinates and temperature parameters [91Pil]. The P and O atoms are on the special positions (0, 0, 0) and (0, 0, 1/2), respectively, which constrains U_{ij} to $U_{22} = U_{11}$ and $U_{12} = U_{13} = U_{23} = 0$. Temperature parameters U_{ij} are defined by Eq. (d) in Introduction. The fractional coordinates and temperature parameters have been multiplied by 10^4, the unit of the thermal parameters being $Å^2$. AP: atmospheric pressure. HP: high pressure of $8.9 \cdot 10^8$ Pa.

		DADP, AP	ADP, AP	ADP, HP			DADP, AP	ADP, AP	ADP, HP
P	U_{11}	118(8)	64(2)	66(4)	D(N)	x	1078(14)	1099(7)	1103(6)
	U_{33}	168(9)	112(4)	112		y	144(14)	159(6)	152(7)
N	U_{11}	244(6)	160(2)	138(4)		z	5775(9)	5758(4)	5794(31)
	U_{33}	154(5)	98(3)	98		U_{11}	801(27)	516(10)	453(18)
O	x	1476(3)	1479(1)	1486(2)		U_{22}	353(14)	302(7)	316(15)
	y	831(2)	846(1)	849(2)		U_{33}	548(15)	407(10)	407
	z	1159(3)	1152(1)	1160(10)		U_{12}	7(29)	20(9)	55(15)
	U_{11}	169(5)	105(2)	105(4)		U_{13}	–457(18)	–290(10)	–290
	U_{22}	150(5)	91(2)	87(4)		U_{23}	–51(19)	–70(12)	–70
	U_{33}	259(6)	159(3)	159	D(O)	x	1432(7)	1446(4)	1465(7)
	U_{12}	21(10)	16(1)	12(3)		y	2205(5)	2268(3)	2307(9)
	U_{13}	–78(12)	–53(2)	–53		z	1182(6)	1194(7)	1304(59)
	U_{23}	–51(4)	–34(2)	–34		U_{11}	204(11)	193(8)	211(13)
						U_{22}	193(15)	203(12)	211
						U_{33}	225(12)	215(11)	211
						U_{12}	66(24)	–1(5)	0
						U_{13}	–88(31)	30(30)	0
						U_{23}	–20(13)	–39(16)	0

Table 33A-5-008. $ND_4D_2PO_4$ (DADP). Fractional coordinates of deuterium in O–D...O [73Hew]. $T = 295$ K and 77.4 K.

	$T = 295$ K				$T = 77.4$ K			
	x	y	z	Occupation	x	y	z	Occupation
D(O, 1)	0.277(3)	0.144(1)	0.140(4)	1/2	0.275(3)	0.144(3)	0.134(3)	1
D(O, 2)	0.223	0.144	0.110	1/2				0
D(O, 3)	–0.144	0.277	–0.140	1/2	–0.146(3)	0.277(3)	–0.145(3)	1
D(O, 4)	–0.144	0.223	–0.110	1/2				0

Table 33A-5-009. $NH_4H_2PO_4$ (ADP), $NH_4H_2AsO_4$ (ADA). Interatomic distances and angles at RT [73Kha]. O(u) and O(l) represent, respectively, the upper and the lower oxygen atoms of a given tetrahedral group as viewed along the *c* axis. O(f) and O(s) represent, respectively, the oxygen atoms of the flat and steep disphenoids around the N atoms.

		$NH_4H_2PO_4$(ADP)	$NH_4H_2AsO_4$(ADA)
4×	X–O(X = P or As)	1.537 (1) Å	1.682 (1) Å
4×	O(u)–X–O(u)	111.17 (4)°	111.08 (7)°
2×	O(u)–X–O(l)	108.63 (4)	108.67 (6)
2×	O(u)–O(u)	2.536 (1) Å	2.774 (2) Å
4×	O(u)–O(l)	2.497 (1)	2.733 (2)
	O–H···O	2.490 (1)	2.512 (2)
4×	N–H···O(f)	2.909 (1)	2.889 (1)
4×	N–H···O(s)	3.170 (1)	3.220 (2)
4×	O(f)–N···O(f)	97.04 (2)°	96.58 (4)°
2×	O(f)–N···O(f)	139.01 (2)	140.42 (5)
2×	O(s)–N···O(s)	47.16 (2)	50.92 (4)
4×	O(s)–N···O(s)	147.14 (2)	144.60 (4)

Table 33A-5-010. $NH_4H_2PO_4$ (ADP), $NH_4H_2AsO_4$ (ADA). Root mean square thermal displacements along principal axes of the thermal ellipsoid and their orientation relative to the crystallographic axes at RT [73Kha].

	Axis	Displacement	[100]	[010]	[001]
$NH_4H_2PO_4$(ADP)					
P	1	0.126 (1) Å	0°	90°	90°
	2	0.126	90	0	90
	3	0.156 (1)	90	90	0
N	1	0.156 (3)	90	90	0
	2	0.177 (2)	0	90	90
	3	0.177	90	0	90
O	1	0.130 (1)	86 (7)	33 (3)	57 (2)
	2	0.138 (1)	161 (2)	77 (7)	103 (4)
	3	0.208 (1)	108 (1)	120 (1)	36 (1)
$NH_4H_2AsO_4$(ADA)					
As	1	0.131 (1) Å	0°	90°	90°
	2	0.131	90	0	90
	3	0.164 (1)	90	90	0
N	1	0.164 (3)	90	90	0
	2	0.183 (2)	0	90	90
	3	0.183	90	0	90
O	1	0.135 (2)	106 (7)	29 (2)	67 (3)
	2	0.143 (2)	155 (5)	97 (7)	114 (3)
	3	0.235 (2)	108 (1)	108 (1)	34 (1)

Table 33A-5-011. $NH_4H_2PO_4$ (ADP). Dielectric constants for some frequencies at RT [61Rus].

f	$\varkappa_a$	$\varkappa_c$	T [°C]
10 kHz	57.6 (5)	14.0 (2)	18.5
1 MHz	57.2 (6)		21.5
1 MHz		14.0 (2)	21
36 GHz	57.1 (6)		21.5
36 GHz		14.0 (3)	21

Table 33A-5-012. $NH_4H_2PO_4$ (ADP), $ND_4D_2PO_4$ (DADP). Piezoelectric constants [66Bec].

Crystals	d_{14}	d_{36}	e_{14}	e_{36}	g_{14}	g_{36}	h_{14}	h_{36}	k_{36}	T	Ref.
	[$\cdot 10^{-12}$ C N^{-1}]		[C m^{-2}]		[$\cdot 10^{-3}$ m^2 C^{-1}]		[$\cdot 10^{8}$ N C^{-1}]			[°C]	
$NH_4H_2PO_4$	1.51	–45.6								20	38Spi
(ADP)		48								27	48Jaf
	1.3	48								RT	61Jaf
			0.015	0.319	3.1	375	0.27	26.3		0	50Van
			0.015	–0.294						20	57Bec
									0.32		62Ber
		43.2		0.254		354		22.4		100	46Mas
		44.2		0.261		348		22.6		80	
		45.3		0.271		348		23.0		60	
		47.3		0.287		353		23.6		40	
		49.3		0.301		356		24.3		20	
		51.7		0.318		360		25.1		0	
		54		0.333		354		25.3		–20	
		57		0.355		363		26.2		–40	
		60		0.377		366		26.8		–60	
		66		0.413		375		28.1		–80	
		69		0.43		384		28.8		–100	
		81		0.50		390		30.0		–110	
		87		0.51		396		30.6		–120	
		90		0.52		396		30.9		–122	
$ND_4D_2PO_4$	10	75								20	62Gar
(DADP)											

Table 33A-5-013. $NH_4H_2PO_4$ (ADP), $ND_4D_2PO_4$ (DADP). Elastic constants [66Bec].

Crystals	s_{11}	s_{12}	s_{13}	s_{33}	s_{44}	s_{66}	T [°C]	Ref.
	[$\cdot 10^{-11}$ m^2 N^{-1}]							
$NH_4H_2PO_4$					11.6	16.6	20	45Jaf
	1.75	0.75	–1.15	4.35	11.5	16.4	25	46Mas
	2.00	0.17	–1.29	4.57	11.70	18.5	20	46Zwi
	1.81	0.19	–1.18	4.35	11.53	16.46	20	57Bec
$ND_4D_2PO_4$	1.9	0.2	–1.15	4.4	11.0	16.4	20	52Mas
	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}		
	[$\cdot 10^{10}$ N m^{-2}]							
$NH_4H_2PO_4$	7.57	–2.43	1.30	2.96	0.87	0.61	25	46Mas
	6.17	0.72	1.94	3.28	0.85	0.592	20	46Zwi
	6.89	0.40	1.89	3.35	0.856	0.595		50Pri
	6.76	0.59	2.00	3.38	0.87	0.61	20	57Bec
	6.80			3.42	0.862	0.602		62Ale
	6.877	0.406	2.038	3.402	0.862	0.601	20	64Hau
$ND_4D_2PO_4$	6.28	0.395	1.74	3.18	0.909	0.610	RT	52Mas

Table 33A-5-014. $NH_4H_2PO_4$ (ADP). n vs. λ [64Zer]. T = 24.8 °C.

λ [μm]	Index in air		Absolute index	
	n_o	n_e	n_o	n_e
0.2000	1.648335	1.587012	1.649083	1.587632
0.3000	1.563478	1.512318	1.563951	1.512787
0.4000	1.540308	1.492136	1.540785	1.492571
0.5000	1.529792	1.483315	1.530276	1.483737
0.6000	1.523539	1.478412	1.524024	1.478828
0.7000	1.519047	1.475202	1.519528	1.475614
0.8000	1.515340	1.472818	1.515813	1.473227
0.9000	1.511969	1.470859	1.512433	1.471268
1.0000	1.508705	1.469123	1.509156	1.469530
1.1000	1.505418	1.467494	1.505853	1.467901
1.2000	1.502029	1.465904	1.502447	1.466311
1.3000	1.498490	1.464311	1.498888	1.464718
1.4000	1.494766	1.462687	1.495142	1.463094
1.5000	1.490834	1.461012	1.491187	1.461419
1.6000	1.486676	1.459272	1.487004	1.459679
1.7000	1.482279	1.457458	1.482580	1.457865
1.8000	1.477631	1.455562	1.477903	1.455970
1.9000	1.472724	1.453578	1.472965	1.453986
2.0000	1.467548	1.451501	1.467756	1.451910

Table 33A-5-015. $NH_4H_2PO_4$ (ADP). n_o, n_e with respect to air vs. λ [87Kir]. T = 33.0(4) °C. IF: narrow-band interference filter.

λ [Å]	Source	n_o	n_e
4046.56	Hg	1.53885	1.49141
4358.33	Hg	1.53497	1.48810
4678.15	Cd	1.53171	1.48540
4799.91	Cd	1.53065	1.48452
5085.82	Cd	1.52835	1.48268
5460.74	Hg	1.52588	1.48062
5893.0	Na	1.52331	1.47875
6438.47	Cd	1.52076	1.47678
7800.27	Rb	1.51534	1.47316
7947.60	Rb	1.51490	1.47278
8521.13	Cs	1.51285	1.47155
8943.46	Cs	1.51143	1.47078
10640.00	Xe +IF	1.50866	1.46795

Table 33A-5-016. $ND_4D_2PO_4$ (DADP). n_o, n_e with respect to air vs. λ [87Kir]. T = 33.0(4) °C. IF: narrow-band interference filter.

λ [Å]	Source	n_o	n_e
4046.56	Hg	1.53216	1.47380
4358.33	Hg	1.52858	1.48419
4678.15	Cd	1.52546	1.48162
4799.91	Cd	1.52450	1.48080
5085.82	Cd	1.52241	1.47898
5460.74	Hg	1.52027	1.47713
5790.66	Hg	1.51862	1.47575
6438.47	Cd	1.51564	1.47337
7800.27	Rb	1.51152	1.47019
7947.60	Rb	1.51112	1.46992
8521.13	Cs	1.50969	1.46894
8943.46	Cs	1.50868	1.46824
10640.00	Xe + IF	1.50497	1.46593

Table 33A-5-017. $NH_4H_2PO_4$ (ADP). Electrooptic constants.

r_{41}^{T}	r_{41}^{S}	r_{63}^{T}	r_{63}^{S}	T	λ	Ref.
[$\cdot 10^{-12}$ m V^{-1}]				[°C]	[nm]	
20.8		8.47		22	556	66Bec
24.5				RT	546	
		8.73		RT	408	
		8.66			436	
		8.62			468	
		8.59			492	
		8.56			546	
		8.54			579	
		8.49			623	
		8.48			500	
		8.4			500	
24.42					405	69Bec
24.27					436	
24.26					492	
23.76					546	
23.32					578	
23.67					611.8	
23.41					632.8	
23.38					730.6	
22.65					1080	
–22.18	–22.03	6.96	11.43	21	589	76Vee

Table 33A-5-018. $NH_4H_2PO_4$ (ADP). Electrooptic constants r_{63}, ρ_{63} vs. T [51Car, 66Bec]. $\lambda = 546$ nm.

T [°C]	r_{63}^{T}	r_{63}^{S}	ρ_{63}^{T}	ρ_{63}^{S}
	[$\cdot 10^{-12}$ m V^{-1}]		[$\cdot 10^{-3}$ m^2 C^{-1}]	
–120	–15.7	–8.33	–74.7	–50.7
–110	–15.0	–7.97	–77.4	–51.3
–100	–14.4	–7.60	–78.6	–51.0
–90	–13.7	–7.27	–79.2	–50.7
–80	–13.1	–7.03	–79.2	–50.7
–70	–12.5	–6.67	–78.0	–49.2
–60	–11.9	–6.40	–76.8	–48.6
–50	–11.3	–6.10	–75.0	–46.8
–40	–10.8	–5.80	–73.2	–45.9
–30	–10.3	–5.60	–71.4	–44.7
–20	–9.87	–5.37	–70.2	–43.5
–10	–9.50	–5.23	–69.0	–43.2
0	–9.13	–5.03	–67.8	–42.3
10	–8.80	–4.87	–66.6	–41.7
20	–8.57	–4.77	–66.0	–41.4
30	–8.33	–4.63	–65.7	–40.8

Table 33A-5-019. $NH_4H_2PO_4$ (ADP). Piezooptic constants.

$\Pi_{11}-\Pi_{12}$	Π_{11}	Π_{12}	Π_{13}	Π_{31}	Π_{33}	Π_{44}	Π_{66}	T	λ	Ref.
[$\cdot 10^{-12}$ m^2 N^{-1}]								[°C]	[nm]	
							–18.0			59Smi
							–18.15		560	48Wes
							–12.5			50Wil
0.7	8.6	7.9		12.3		–5.8	–12.2			54Car
							–13.6			59Jaf
0.78						5.78*)	19.6*)			55Dev
1.04							–18.15			50Wes
			–37.3		35.7			RT		61Ach
	4.40	3.71	0.34	2.02	2.65	–6.70	–15.25	21	589	73Nar
$\frac{1}{2}(p_{11}-p_{12})$	p_{11}	p_{12}	p_{13}	p_{31}	p_{33}	p_{44}	p_{66}			
Dimensionless										
0.052							–0.1107		560	50Wes
							–0.0744			54Car
							–0.076			50Wil
	–0.11	–0.15	–0.93	0.20	–0.71			RT		61Ach
	0.302*)	0.246*)	0.236*)	0.195*)	0.263*)		0.075*) (p_{66}^{E})		633	67Dix
	0.319	0.277	0.169	0.197	0.167	–0.058	–0.091	21	589	73Nar
	0.292*)	0.243*)		0.185*)				22	633	73Mar
	0.296*)	0.243*)	0.208*)	0.188*)	0.228*)				633	77Ale

*) Absolute value.

Table 33A-5-020. $NH_4H_2PO_4$ (ADP). Piezooptic constants Π_{66} and p_{66} for various T [51Car, 66Bec]. $\lambda = 546$ nm.

T	Π_{66}^{E}	Π_{66}^{D}	Π_{66}^{P}	p_{66}^{E}	p_{66}^{D}	p_{66}^{P}
[°C]	[$\cdot 10^{-12}$ m^2 N^{-1}]			[$\cdot 10^{-2}$]		
–120	–14.0	–7.8	–7.5	–8.5	–6.0	–5.8
–110	–14.4	–8.5	–8.3	–8.9	–6.5	–6.4
–100	–14.9	–9.4	–9.1	–9.2	–7.0	–6.9
–90	–15.0	–9.8	–9.6	–9.4	–7.3	–7.2
–80	–14.8	–10.0	–9.6	–9.3	–7.4	–7.3
–70	–14.6	–10.1	–9.7	–9.3	–7.4	–7.3
–60	–14.4	–10.0	–9.7	–9.1	–7.4	–7.3
–50	–14.1	–10.0	–9.7	–8.9	–7.3	–7.2
–40	–13.9	–10.0	–9.7	–8.8	–7.2	–7.1
–30	–13.7	–9.9	–9.7	–8.6	–7.1	–7.0
–20	–13.5	–9.7	–9.6	–8.4	–7.0	–6.9
–10	–13.0	–9.6	–9.5	–8.1	–6.8	–6.7
0	–12.9	–9.6	–9.4	–8.0	–6.7	–6.7
10	–12.8	–9.6	–9.4	–7.9	–6.6	–6.6
20	–12.6	–9.6	–9.4	–7.7	–6.5	–6.5
30	–12.6	–9.6	–9.5	–7.7	–6.6	–6.5

Table 33A-5-021. $ND_4D_2PO_4$ (DADP), $NH_4H_2PO_4$ (ADP). NMR data of acid D, ammonium D and ^{14}N. η: asymmetry parameter. F.g.: field gradient tensor. q_I, q_{II}, q_{III} are defined as the principal components of the F.g. tensor with $|q_I| > |q_{II}| > |q_{III}|$.

T [°C]	Crystals	Nuclei	$e^2 qQ/h$ [kHz]	η	Remarks	Ref.
RT	$NH_4H_2PO_4$	^{14}N	24.6	0	F. g. $\parallel c$	65Chi
RT	$ND_4D_2PO_4$	^{14}N	27.3			65Chi
RT		D (acid)	119.6(8)	0.053(8)	q_I in a-axis, q_{II} in c-axis q_{III} in a-axis directions	64Chi
RT		D (ammonium)	3.4	0	F. g. $\parallel c$	65Chi
–40		D (ammonium)	6.0	0.89	F. g. *)	65Chi

*)

F. g. component	a (or b)	b (or a)	c
Z	0.226	0.413	0.882
Y	0.681	0.580	–0.447
X	–0.696	0.702	–0.150

And three other sets of F. g. direction cosines which differ from the one listed by the sign of either a, or b, or c axis component.

Table 33A-5-022. $ND_4D_2PO_4$ (DADP). Principal components of deuteron quadrupole coupling tensors ($eQ\phi_{ii}/h$) and their orientations in parenthesis. θ and ϕ are directions of principal axes of quadrupole-coupling tensor relative to the crystal axes in a $I\bar{4}2d$ cell.

T [°C]	Type	$\lvert eQ\phi_{zz}/h \rvert$ (θ_z, ϕ_z) [kHz]	$\lvert eQ\phi_{yy}/h \rvert$ (θ_y, ϕ_y)	$\lvert eQ\phi_{xx}/h \rvert$ (θ_x, ϕ_x)	Ref.
25	x	118 (90°, – 2°)	62 (2°, – 96°)	56 (92°, – 92°)	68Gen
	y	120 (90°, – 93°)	61 (6°, – 179°)	59 (84°, – 3°)	
–65		131 (90°, 0°)	72 (25°, 90°)	59 (65°, – 90°)	
25		120 (90°, 0°)	63 (0°, –)	57 (90°, 90°)	
–70		128.2(15)	71.0(15)	57.2(15)	74Bli
		η = 0.108(10)			

Table 33A-5-023. $ND_4D_2PO_4$ (DADP). Direction cosines of the largest principal values of the 16 physically nonequivalent O–D...O deuteron electric field gradient tensors below Θ_{II-I} [74Bli].

O – D···O bonds along the *a* direction								
	Domain A				Domain B			
a	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
b	0.083	–0.083	0.083	–0.083	0.028	–0.028	0.028	–0.028
c	0.028	0.028	–0.028	–0.028	0.083	0.083	–0.083	–0.083
O – D···O bonds along the *b* direction								
	Domain A				Domain B			
a	0.083	–0.083	0.083	–0.083	0.028	–0.028	0.028	–0.028
b	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
c	0.028	0.028	–0.028	–0.028	0.083	0.083	–0.083	–0.083

Table 33A-5-024. $NH_4H_2PO_4:Cr^{3+}$. Spin Hamiltonian parameters and direction cosines of the principal Z axis with respect to the a, b, and c axes at 215 K [78Die]. $B_2^0 = D/3$, $B_2^2 = E$, in units of 10^{-2} m^{-1}. Three solutions are shown. See also [70Kaw].

	a	b	c
B_2^0	–385	49	336
B_2^2	–287	–721	434
$g_{xx}=g_{yy}=g_{zz}$	1.97	1.97	1.97
l*)	0.540 (57.3)	–0.744 (138.1)	0.003 (89.8)
m*)	0.810 (35.9)	–0.586 (125.9)	–0.276 (106.2)
n*)	–0.227 (103.1)	0.321 (71.2)	0.961 (16.1)

*) l, m, and n are the direction cosines of the principal Z-axis with respect to the a-, b-, and c-axis, respectively (in parentheses the corresponding angles in degrees of arc).