Table 38A-1-001. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Fractional coordinates of atoms [84Ave].

Atoms	x	y	z	Atoms	x	y	z
Te	0	0.0015(2)	0	O(6)	0.0705(8)	0.5158(15)	0.2651(13)
P(1)	0.1323(3)	0.5385(7)	0.4104(5)	O(7)	0.9198(6)	0.7679(14)	0.9455(10)
P(2)	0.7504(4)	0.0056(2)	0.2500(8)	O(8)	0.6876(7)	0.6586(18)	0.9504(11)
P(3)	0.3701(3)	0.5380(6)	0.0906(5)	O(9)	0.5350(8)	0.9995(14)	0.3304(13)
N(1)	0.2456(11)	0.0776(7)	0.2527(17)	O(10)	0.4219(8)	0.5762(21)	0.9823(13)
N(2)	0.6175(6)	0.5237(17)	0.3281(10)	O(11)	0.7078(6)	0.1280(17)	0.3501(11)
N(3)	0.8818(9)	0.5412(22)	0.1763(15)	O(12)	0.0756(7)	0.2456(15)	0.0549(12)
N(4)	0.4990(24)	0.0152(33)	0.9989(44)	O(13)	0.3006(7)	0.3595(19)	0.0403(11)
O(1)	0.8293(2)	0.8725(6)	0.3472(4)	O(14)	0.9647(8)	0.0248(16)	0.1772(14)
O(2)	0.6949(2)	0.2701(6)	0.9090(4)	O(15)	0.5761(8)	0.4306(21)	0.0200(12)
O(3)	0.9006(4)	0.1826(12)	0.9178(9)	O(16)	0.6803(2)	0.8479(6)	0.1692(4)
O(4)	0.0964(6)	0.8265(19)	0.0931(11)	O(17)	0.7903(7)	0.1425(17)	0.1562(12)
O(5)	0.4265(8)	0.5090(15)	0.2421(13)	O(18)	0.3209(3)	0.7583(6)	0.0880(4)

Table 38A-1-002. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Anisotropic temperature parameters [$\cdot 10^{-4}$] of atoms [84Ave]. b_{ij} are defined by Eq. (b) in Introduction.

Atoms	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Te	10.51(8)	72.3(5)	26.5(2)	−0.6(3)	5.02(9)	4.6(4)
P(1)	21(2)	134(10)	39(5)	−3(4)	6(2)	14(6)
P(2)	13.1(3)	73(2)	33.2(7)	4(4)	7.1(4)	22(6)
P(3)	16(2)	62(7)	26(4)	−2(3)	5(2)	−3(4)
N(1)	17(3)	159(9)	60(4)	15(7)	8(3)	66(14)
N(2)	12(3)	84(17)	30(7)	−4(7)	9(4)	21(10)
N(3)	43(5)	147(27)	84(14)	−19(11)	5(7)	57(17)
N(4)	62(4)	141(24)	145(7)	28(10)	−5(4)	41(18)
O(1)	15(1)	97(9)	38(4)	16(3)	3(2)	23(5)
O(2)	21(2)	134(10)	29(3)	13(3)	−1(2)	−3(5)
O(3)	3(2)	62(13)	41(7)	3(4)	5(3)	39(8)
O(4)	30(4)	207(26)	63(10)	21(8)	15(5)	9(13)
O(5)	20(4)	135(27)	33(8)	11(8)	6(4)	−25(11)
O(6)	21(4)	103(24)	43(10)	3(7)	−1(5)	−29(11)
O(7)	15(3)	96(16)	29(7)	7(5)	5(3)	−14(8)
O(8)	41(4)	156(19)	46(7)	−37(7)	24(4)	−23(9)
O(9)	19(3)	105(15)	19(7)	−4(5)	8(4)	8(7)
O(10)	28(5)	153(28)	66(13)	−24(10)	13(6)	−10(15)
O(11)	14(3)	106(18)	35(7)	−1(6)	3(4)	−21(9)
O(12)	25(4)	84(17)	83(10)	−30(6)	19(5)	12(10)
O(13)	18(2)	157(19)	55(7)	−16(5)	7(3)	−30(9)
O(14)	17(3)	133(18)	44(8)	3(5)	14(4)	−3(8)
O(15)	27(4)	215(29)	44(11)	0(9)	24(6)	18(14)
O(16)	23(2)	110(9)	56(4)	−5(3)	9(2)	−5(5)
O(17)	21(4)	96(19)	52(9)	−10(6)	19(4)	9(10)
O(18)	27(2)	103(9)	53(4)	4(3)	9(2)	−2(5)

Table 38A-1-003. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Interatomic distances [Å] and bond angles [°] in PO_4 tetrahedra [84Ave].

PO_4				
P(1)	O(2)	O(6)	O(8)	O(15)
O(2)	1.559(6)	2.48(1)	2.49(1)	2.60(1)
O(6)	108.2(6)	1.502(12)	2.47(1)	2.50(2)
O(8)	108.8(5)	110.4(7)	1.508(12)	2.49(2)
O(15)	112.2(6)	109.0(7)	108.2(7)	1.572(15)
P(2)	O(1)	O(11)	O(16)	O(17)
O(1)	1.586(6)	2.50(1)	2.519(4)	2.49(1)
O(11)	106.5(5)	1.536(13)	2.46(1)	2.579(2)
O(16)	107.6(4)	106.5(5)	1.536(6)	2.56(1)
O(17)	106.6(5)	115.0(6)	114.2(5)	1.515(14)
P(3)	O(5)	O(10)	O(13)	O(18)
O(5)	1.524(12)	2.57(2)	2.57(1)	2.48(1)
O(10)	115.0(7)	1.519(15)	2.53(2)	2.40(1)
O(13)	113.5(6)	110.6(7)	1.553(12)	2.57(1)
O(18)	105.9(5)	101.3(6)	109.6(5)	1.587(5)

Table 38A-1-004. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Interatomic distances [Å] and bond angles [°] in TeO_6 octahedron and NO_n polyhedra [84Ave].

TeO_6						
Te	O(3)	O(4)	O(7)	O(9)	O(12)	O(14)
O(3)	1.927(7)	3.82(1)	2.64(1)	2.73(2)	2.74(1)	2.67(1)
O(4)	176.1(4)	1.897(10)	2.78(1)	2.73(2)	2.68(2)	2.72(2)
O(7)	86.8(4)	93.7(4)	1.918(9)	2.79(2)	3.85(1)	2.73(1)
O(9)	91.5(4)	92.4(5)	94.3(5)	1.887(14)	2.63(2)	3.85(2)
O(12)	90.5(4)	88.9(5)	177.1(4)	87.0(5)	1.931(10)	2.74(2)
O(14)	86.5(4)	89.6(5)	89.2(4)	175.9(5)	89.4(5)	1.967(14)

NO_n								
N(1)–O(2)	2.91(1)	N(2)–O(5)	2.89(1)	N(3)–O(1)	2.93(2)	N(4)–O(1)	2.77(3)
–O(3)	3.02(1)	–O(9)	3.27(1)	–O(6)	2.85(2)	–O(9)	3.15(4)
–O(4)	2.91(2)	–O(11)	2.85(1)	–O(7)	2.87(2)	–O(10)	3.01(3)
–O(7)	3.04(2)	–O(12)	2.88(2)	–O(8)	3.33(2)	–O(14)	3.07(4)
–O(8)	2.88(2)	–O(13)	3.15(1)	–O(10)	2.99(2)	–O(15)	2.87(3)
–O(12)	3.04(2)	–O(15)	2.98(2)	–O(14)	3.32(2)	–O(16)	3.07(3)
–O(13)	3.04(2)	–O(16)	2.90(1)	–O(17)	2.88(2)		
–O(18)	3.02(2)						

Table 38A-1-005. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Linear thermal expansion coefficients α_{ij} [$\cdot 10^{-6}$ K^{-1}] [85Hau]. α_{ii}* are the values in the principal axial system.

T [K]	α_{11}	α_{22}	α_{33}	α_{13}	α_{11}*	α_{22}*	α_{33}*
300	7(2)	23(3)	20(3)	–31(4)	–18	23	45
340	25(2)	53(4)	33(3)	–29(4)	–0.3	53	58

Table 38A-1-006. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Elastic stiffness $c_{\lambda\mu}$ [$\cdot 10^{10}$ N m^{-2}] [85Hau]. Parameter: T. f = 6…40 MHz.

T [K]	c_{11}	c_{22}	c_{33}	c_{12}	c_{23}
283	4.557(12)	4.513(12)	4.432(12)	2.662(20)	2.137(20)
293	4.532(12)	4.478(12)	4.406(12)	2.658(20)	2.123(20)
333	4.396(12)	4.522(12)	4.332(12)	2.557(20)	1.822(20)
T [K]	c_{13}	c_{44}	c_{55}	c_{66}	c_{15}
283	1.445(10)	1.210(6)	1.149(6)	1.893(7)	0.019(10)
293	1.442(10)	1.186(6)	1.138(6)	1.888(7)	0.037(10)
333	1.436(10)	1.159(6)	1.130(6)	1.840(7)	−0.008(10)
T [K]	c_{25}	c_{35}	c_{46}		
283	−0.288(30)	−0.256(10)	0.494(10)		
293	−0.271(30)	−0.263(10)	0.492(10)		
333	0.482(30)	−0.142(10)	0.490(10)		

Table 38A-1-007. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Parameters of simplified Sellmeier formula, $n_i^2 - 1 = S_i\lambda_i^2\lambda^2/(\lambda^2 - \lambda_i^2)$ [84Gui].

	n_1	n_2	n_3
S_i [(μm)$^{-2}$]	67.94	67.46	65.88
λ_i [μm]	0.1382	0.1382	0.1414

Table 38A-1-008. $Te(OH)_6 \cdot 2NH_4H_2PO_4 \cdot (NH_4)_2HPO_4$ (TAAP). Mode frequencies [cm^{-1}] of Raman and infrared spectra [88Vis]. α_{xx} etc.: polarizability tensor components associated with the scattering geometries for Raman spectra.

Raman [cm^{-1}]						IR	Assignments *
α_{xx}	α_{xz}	α_{yy}	α_{zz}	α_{xy}	α_{yz}	[cm^{-1}]	
91	72	92	98	91	92		
94	92	123	123		98		
126	96						
	121						External modes
144	146	143	144	144	147		ν(N–H…O)
				187			
185	206	201	202	204	207	201 w	
201	256	241	239	254	243	222 w	
231		283		269	291	235 w	
252		301				250 w	
287						262 w	
						290 m	
304	310	316	299	316	310		
316	346	342	342	324		330 m	ν_5 TeO_6
346				346	346		
364	354	356	360	358	357		
	361	363	370		361		ν_4 TeO_6
	374				376		
385	384	384	384	386	384		
439	391	401			396		ν_2 PO_4
	446				417		
514	490	478	496	498	487		
558	502	493	513	507	503	500 br	ν_4 PO_4
567	562	516	530	521	536		
		531	554	564	558		
		558					
586	584	592	587	570	576		
618	638	604	596	607	584		
632		632	631	632	603		ν_2 TeO_6
654	654	654	654	654	654	650 m	ν_1 TeO_6
708	704	729	729	708	711		
716	750	750	764	716	722		
770	786	777		750	733		Combination
				785	759		δ(Te,P)–O–H
					783		
810	820	806	809	830	830		
	849	820					ν P–O(H)
		847					
		875					
930	930	930	930	930	930		
956	956	956	956	956	956	900–950 br	ν_1 PO_4
960	960	960	960	960	960		
1006	1000	1048	1048	1066	1011		
1024	1013	1069	1034	1088	1020	1050–1150 br	ν_3 PO_4
1048	1053	1114	1098	1106	1038		

(continued)

Table 38A-1-008 (continued)

Raman [cm^{-1}]						IR	Assignments *
α_{xx}	α_{xz}	α_{yy}	α_{zz}	α_{xy}	α_{yz}	[cm^{-1}]	
1056	1058	1139	1126	1114	1057		
1069	1071	1164	1188	1140	1073		
1086	1088	1181		1132	1096		
1099	1108			1187	1106		
	1152				1134		
	1180				1133		
1226	1210	1215	1236	1201	1231		β(Te,P)–O–H
			1242				
1448	1406	1423	1476	1444	1406	1400 m	
1464	1423	1456	1528	1458	1446		
1501	1446	1473	1560	1466	1542		
1557	1468	1516		1501			ν_4 NH_4
1571	1540	1538		1528			
	1582			1574			
				1590		1560 w	
1606	1602	1606	1603	1608	1621		
1672	1706	1642	1694	1648	1708		
1710	1734	1664	1725	1674	1764		
1728	1752	1719	1738	1710	1782		
1760	1764	1753	1847	1718		1700 br	ν_2 NH_4
		1768		1724			
1802		1787		1758			
1830		1810		1784			
2810	2820	2866	2909	2896	2896		
2837	2868	2899		2902			
2903	2890	2905				2900 br	Combination
		2919					ν(Te,P)–OH
	2933	2947	2947		2944		
		2986					
3008	3084	3006	3015	3000	3020		
3017	3097	3084	3031	3062	3099	3100 br	ν_1 NH_4
3024	3124	3143	3040	3084	3121		
3052	3200	3154	3070	3124	3188		ν_3 NH_4
3069		3244	3090	3182			
3114			3128	3220			
3158			3186				
3208			3206				
			3270				

* ν: Stretching. β: in plane bending. δ: out of plane bending.