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A Redetermination of the Crystal Structure of $KTeO_3(OH)$

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The crystal structure of $KTeO_3(OH)$ has been reinvestigated. $KTeO_3(OH)$ crystallizes in space group $P2_1/a$ with $a = 6.498$, $b = 11.696$, $c = 5.121$ Å, and $\beta = 93.86°$ and with $Z = 4$. The refinement of the atomic parameters was based on 3706 single-crystal X-ray reflections, collected with a Philips Pailred diffractometer, a final R value of 0.044 being obtained. The structure contains $Te-O_6$ octahedra which share edges, thus forming infinite chains. Apart from the electrostatic forces due to the potassium ions, the $[TeO_3(OH)]_n^{n-}$ chains are held together by strong hydrogen bonds with distances of 2.480 Å. The coordination distances around tellurium are: $Te-O_{bridge} = 1.945$, 1.947, 1.994, and 1.997 Å, $Te-OH = 1.883$ Å and $Te-O = 1.843$ Å.

A characteristic feature of tellurates containing both Te–OH and Te–O (terminal) bonds is that the Te–O bond distance is about 0.1 Å shorter than the Te–OH bond distance. This difference usually makes it possible to distinguish between the two types of bond in an ordinary X-ray investigation, although in the compounds $KTeO_2(OH)_3$ [1] and $KTeO_3(OH)$ [2] these two bond lengths are equal owing to symmetry. However, the structure of $KTeO_2(OH)_3$ given by Lammers and Zemann was idealized, and, as they pointed out,[1] there ought to be slight deviations from ideality. It therefore seems reasonable to assume that the Te–OH bond is in fact longer than the Te–O bond. Lammers, who determined the structure of $KTeO_3(OH)$ using data from three film projections, found systematic absences according to the centric space group $I2/a$.[2] Apart from yielding equal Te–OH and Te–O bond distances, this symmetry implies either disordered hydrogen atom positions or the presence of a symmetrical hydrogen bond. The latter would, however, seem unlikely in view of the O–O hydrogen bond distance of 2.62 Å reported by Lammers.

In cooperation with Dr. Jan Petrovič, Slovac Academy of Sciences, Bratislava, a series of hydrothermal experiments was performed, in 1969, on aqueous solutions of $Te(OH)_6$, KOH and K_2CO_3 mixed in different proportions. In one of the preparations well-developed crystals of $KTeO_3(OH)$ were obtained. Since a preliminary X-ray investigation showed the space group to be

$P2_1/a$, rather than $I2/a$, with the orientation given by Lammers, it was decided to perform a reinvestigation of the crystal structure of $KTeO_3(OH)$.

EXPERIMENTAL

Crystals of $KTeO_3(OH)$ were prepared according to the method described by Lammers and Zemann.[1,2] In one preparation large colourless needles with lengths up to 3 mm were obtained.

Preliminary Weissenberg exposures of the layers $hk0$ and $hk1$ showed the crystals to be monoclinic with cell dimensions in agreement with the values previously given by Lammers. However, the only systematic absences found were: $h0l$ with $h=2n+1$ and $0k0$ with $k=2n+1$, indicating the space group to be $P2_1/a$ rather than $I2/a$. Although all reflections with $h+k+l$ odd were generally much weaker than those with $h+k+l$ even, a large number of such reflections were clearly visible on the films.

Table 1. Cell dimensions and powder data for $KTeO_3(OH)$.

$a = 6.4981(5)$ Å
$b = 11.696(1)$ Å
$c = 5.1210(3)$ Å
$\beta = 93.861(6)°$
$V = 388.33(5)$ Å^3
$Z = 4$

$h\ k\ l$	$\sin^2\theta \times 10^5$ obs.	$\sin^2\theta \times 10^5$ calc.	$h\ k\ l$	$\sin^2\theta \times 10^5$ obs.	$\sin^2\theta \times 10^5$ calc.
0 2 0	1736	1735	−1 2 3	22869	22876
−1 1 0	1840	1845	−3 5 0	23535	23545
0 1 1	2702	2706	3 1 2	23657	23674
−1 2 1	5174	5178	0 3 3	24336	24357
−1 3 0	5311	5314	0 6 2	24702	24703
1 2 1	5652	5660	−4 3 1	27769	27794
0 3 1	6175	6176	−1 4 3	28072	28080
0 4 0	6937	6939	−2 3 3	28551	28555
−2 2 0	7382	7380	1 4 3	29523	29528
0 0 2	9091	9091	−4 0 2	29723	29744
−1 1 2	10450	10453	−1 7 2	31268	31270
0 2 2	10817	10825	1 7 2	32215	32234
1 4 1	10856	10864	−3 2 3	32716	32721
−2 3 1	11335	11339	−2 8 0	33399	33401
1 1 2	11419	11418	−3 7 0	33949	33953
−1 5 0	12244	12253	−4 5 1	34728	34733
2 3 1	12301	12304	−2 5 3	35493	35494
0 5 1	13106	13114	5 1 0	35732	35719
−2 0 2	13772	13772	0 0 4	36363	36362
1 3 2	14877	14887	−1 1 4	37245	37243
−2 2 2	15497	15506	0 9 1	37396	37400
2 0 2	15692	15701	0 2 4	38106	38097
−3 2 1	15980	15987	1 1 4	39167	39172
−3 3 0	16599	16606	5 2 1	40485	40499
3 2 1	17432	17434	−2 8 2	41531	41527
−3 1 2	20765	20780	2 0 4	43928	43938
−1 5 2	20847	20861	3 7 2	44500	44491
−3 4 1	21204	21191	−3 1 4	46607	46605
2 6 0	21240	21258	5 1 2	47219	47222
1 5 2	21811	21826	−1 5 4	47625	47651
3 4 1	22633	22638			

To obtain accurate cell dimensions, a Guinier powder photograph was taken, using lead nitrate as an internal standard ($a_{Pb(NO_3)_2} = 7.8566$ Å at 21°C).[3] The cell parameters were refined with the program POWDER [4] and the results are shown in Table 1.

Table 2. Boundary planes and corresponding distances from an internal origin for the crystal used in the investigation.

h	k	l	d (mm)
1	0	0	0.050
−1	0	0	0.050
1	6	0	0.034
−1	−6	0	0.034
−1	2	0	0.044
0	0	1	0.233
0	0	−1	0.233

A crystal of the dimensions given in Table 2 was mounted along the needle axis (c axis) in a Philips Pailred linear diffractometer. The intensities were recorded with graphite monochromated Mo$K\alpha$ radiation using the ω-scan technique. The background was measured at both ends of the scan interval. The levels $hk0 - hk8$ were measured up to $\sin\theta/\lambda \sim 1.3$ and those 3740 reflections with $\sigma(I)/I < 0.5$ were used in the subsequent calculations. The counting statistics and the Lp correction were calculated with the program DATAP1.[5]

When collecting data from the $hk1$ and $hk3$ layers, five very weak $h01$ and $h03$ reflections with $h = 2n + 1$ were registered (−301, −101, 101, 301, −103). The precise alignment in the Pailred instrument could favour the generation of Renninger reflections, and an examination of pairs of the strongest reflections showed that of the "un-allowed" $h0l$ reflections the five above-mentioned were those most likely to arise from multiple reflection. That these reflections are indeed Renninger reflections is further supported by the fact that no $h0l$ reflection was registered with $h = 2n + 1$ and $l = 2n$. The formation of such a reflection due to the Renninger effect would have required contributions from pairs in which one reflection had $h + k + l = 2n + 1$. Throughout the structure analysis it was, however, borne in mind that the space group might be $P2_1$ or $P2_1/m$ instead of $P2_1/a$.

The linear absorption coefficient for $KTeO_3(OH)$ in Mo$K\alpha$ radiation, $\mu = 87.4$ cm^{-1}, was calculated from atomic mass absorption coefficients given in the *International Tables*.[3] The absorption correction was performed using the program DATAP2,[6] the crystal being divided into $4 \times 8 \times 8$ Gaussian grid points. The transmission factors varied between 0.44 and 0.58.

REFINEMENT

The atomic coordinates given by Lammers [2] were used as starting values in the refinement. In order to make the positions generated in space group $I2/a$ consistent with the symmetry elements of $P2_1/a$ the origin had to be shifted. The cell used in this investigation was therefore translated ($\frac{1}{4}$, $-\frac{1}{4}$, $-\frac{1}{4}$) from Lammers' original cell.

Isotropic refinement, including separate scale factors for the nine $hk0 - hk8$ levels and an isotropic secondary extinction parameter, gave an R value of 0.063. The corresponding isotropic temperature factors are given in Table 4.

To check the validity of space group $P2_1/a$, the structure was refined for several cycles in $P2_1$. The space group $P2_1/m$ was not considered, since the mirror plane perpendicular to the b axis is not consistent with the basic ar-

rangement in the structure. During full matrix refinement the atomic coordinates converged towards the centric arrangement obtained in $P2_1/a$. Since, moreover, the refinement converged slowly and all parameters had relatively high e.s.d.'s when refined in $P2_1$, it was therefore concluded that the true space was $P2_1/a$, and the five very weak reflections in $h0l$ with $h = 2n+1$ were removed from the data set. Some other of the very weakest reflections also appeared to be in error due to simultaneous reflection since the corresponding calculated structure factors were far too low. 29 such reflections

Table 3. Weight analysis after the last cycle of refinement. The quantities $w\Delta^2$ are normalized sums and N is the number of reflections within each F_o interval.

F_o interval	$w\Delta^2$	N
0.0 – 5.3	1.16	351
5.3 – 7.3	0.95	411
7.3 – 10.0	1.03	365
10.0 – 12.8	1.12	323
12.8 – 17.0	0.95	440
17.0 – 21.5	0.80	372
21.5 – 29.0	0.62	411
29.0 – 37.0	1.25	331
37.0 – 50.0	0.93	303
50.0 – 150.0	1.29	399

$R = \sum|\Delta|/\sum F_o = 0.044$ $(\Delta = F_o - F_c)$.
$R_w = (\sum w\Delta^2/\sum wF_o^2)^{1/2} = 0.059$.

Table 4. Final parameters in $KTeO_3(OH)$. The anisotropic factor is $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$. Standard deviations are given in parentheses.

Atom	x	y	z	B (Å^2)
Te	0.00324(2)	0.42824(1)	0.24981(3)	0.706(6)
K	0.4875(1)	0.6586(1)	0.2344(2)	1.83(2)
O_1	0.1657(3)	0.4543(2)	0.9599(5)	0.97(3)
O_2	0.1546(3)	0.5540(2)	0.4428(4)	0.93(3)
O_3	0.1972(4)	0.3262(2)	0.4098(6)	1.39(4)
O_4	0.1625(4)	0.6862(2)	0.8956(5)	1.24(4)

	$U_{11}\times10^4$	$U_{22}\times10^4$	$U_{33}\times10^4$	$U_{12}\times10^4$	$U_{13}\times10^4$	$U_{23}\times10^4$
Te	100.8(4)	78.1(3)	90.2(6)	4.5(4)	11.5(3)	−1.5(5)
K	150(3)	329(4)	233(4)	−14(2)	1(2)	41(3)
O_1	109(5)	140(7)	119(8)	22(5)	31(5)	5(5)
O_2	132(6)	129(6)	103(8)	−53(5)	37(5)	−21(5)
O_3	244(10)	158(8)	164(10)	111(7)	−35(8)	−5(7)
O_4	231(9)	124(7)	141(9)	−74(6)	3(7)	−11(6)

Extinction parameter:[12] $g = 1.55(4)\times10^4$.
$P2_1/a$, 4(e): $\pm(x,y,z)$, $\pm(1/2-x,1/2+y,-z)$.

Table 5. Observed and calculated structure factors for $KTeO_3(OH)$. The columns are h, $10|F_o|$ and $10|F_c|$, respectively.

H 30 0		
0	87	94
H 28 0		
6	164	182
4	206	218
2	213	224
0	216	228
H 27 0		
1	238	-239
3	220	-225
5	198	-206
7	159	-174
H 26 0		
8	117	129
6	147	150
4	175	171
2	197	196
0	188	185
H 25 0		
1	70	-65
3	85	-88
5	60	-58
7	49	-48
9	53	-50
H 24 0		
9	50	-40
8	54	-49
7	36	-32
6	54	-53
4	68	-60
2	67	-58
H 23 0		
1	198	194
3	228	222
5	147	141
7	100	102
9	45	53
9	131	135
H 22 0		
10	188	-192
9	43	-34
8	272	-264
6	245	-235
4	368	-356
2	398	-393
1	46	-49
0	325	-315
H 21 0		
1	390	386
3	453	449
5	347	345
7	258	256
9	284	284
11	167	177
H 20 0		
12	128	-134
10	242	-240
8	255	-248
6	304	-296
4	416	-402
2	408	-400
0	394	-396
H 19 0		
1	363	368
3	356	357
5	314	312
6	45	-49
7	241	238
9	202	201
10	40	-42
11	161	160
H 18 0		
12	55	-44
11	72	73
10	80	-63
9	52	44
8	90	-81
7	55	51
6	71	-68
5	85	79
4	108	-103
2	135	-137
0	77	-61

H 17 0		
1	178	-177
3	51	-45
4	68	-64
5	151	-148
7	116	-106
9	58	-47
10	42	-44
11	57	-58
12	53	-47
13	46	-47
H 16 0		
14	86	92
13	41	52
12	132	133
11	43	51
10	136	133
9	85	78
8	200	195
7	49	53
6	287	290
5	57	62
4	217	221
3	61	56
2	275	276
0	383	384
H 15 0		
1	692	-693
2	53	-48
3	646	-649
5	497	-499
7	485	-483
8	82	-79
9	337	-337
11	232	-233
13	178	-192
14	44	-47
H 14 0		
14	179	189
12	231	226
10	346	333
8	503	495
6	486	489
4	40	-48
4	685	688
2	826	829
1	47	51
0	662	669
H 13 0		
1	556	-561
3	687	-691
5	447	-456
7	365	-358
9	394	-383
11	229	-225
13	164	-169
15	132	-143
H 12 0		
14	129	130
12	146	149
10	321	306
8	362	354
6	418	414
4	648	654
2	669	676
0	663	672
H 11 0		
1	221	-231
2	62	64
3	227	-233
4	98	95
5	210	-207
6	152	157
7	112	-100
8	119	109
9	150	-142
10	124	125
11	102	-87
12	102	101
14	53	72
15	60	-57
H 10 0		
14	62	-57
12	98	-108
11	102	-82
10	108	-100
9	168	-170
7	43	-40
6	311	-304

5	103	-101
4	288	-283
2	310	-322
0	518	-531
H 9 0		
1	605	621
2	59	-61
3	175	174
4	91	87
5	463	461
6	89	76
7	330	329
9	174	168
11	177	190
13	143	158
15	72	84
H 8 0		
16	101	-113
14	192	-193
12	307	-308
10	345	-344
9	149	-129
8	488	-486
7	127	-108
6	879	-861
5	142	-132
4	792	-775
3	125	-129
2	906	-893
1	57	63
0	1588	-1564
H 7 0		
1	1769	1707
3	1308	1223
5	1122	1083
6	110	-113
7	908	894
9	541	534
11	415	408
13	303	308
15	172	180
H 6 0		
16	117	-122
14	192	-194
12	274	-261
10	311	-310
8	498	-492
7	64	77
6	560	-561
5	93	93
4	719	-711
2	1074	-1013
1	27	-19
0	894	-738
H 5 0		
1	990	958
2	39	38
3	1190	1119
5	607	612
7	506	504
9	393	397
11	242	240
13	135	180
15	87	124
H 4 0		
14	81	-72
13	123	134
12	80	-87
11	103	114
10	184	-186
9	168	178
8	244	-245
7	204	211
6	299	-305
5	121	131
4	544	-548
3	203	205
2	675	-657
1	48	53
0	642	-696
H 3 0		
1	996	-916
2	91	-93
3	838	-814
4	81	-97
5	418	-429
6	132	-140
7	391	-402
8	117	-127

9	203	-206
10	70	-92
11	144	-146
12	121	-100
13	111	-111
14	81	-79
H 2 0		
14	126	138
12	224	225
10	223	223
8	357	369
6	543	554
5	64	54
4	536	547
3	143	-138
2	851	818
0	966	1024
H 1 0		
1	1888	-1762
3	572	-600
4	122	-130
5	964	-968
6	231	-229
7	691	-707
8	101	-90
9	362	-373
10	143	-123
11	348	-344
12	127	-109
13	269	-270
15	134	-148
H 0 0		
16	139	150
14	261	259
12	448	438
10	524	527
8	749	770
6	1441	1449
4	1447	1450
2	1803	1812
H 29 1		
4	81	-93
2	89	-97
0	101	-110
-2	94	-105
-4	81	-91
H 27 1		
0	71	75
4	114	115
3	40	39
2	71	80
1	112	111
-2	99	109
-4	66	75
-6	88	101
H 26 1		
-7	172	-183
-6	38	42
-5	154	-156
-3	178	-181
-1	234	-238
1	180	-185
3	173	-176
5	195	-208
7	121	-129
H 25 1		
8	148	161
6	252	257
4	263	265
2	259	257
0	307	305
-2	302	312
-4	224	235
-6	209	229
-8	205	224
H 24 1		
-9	200	-216
-7	250	-255
-5	257	-263
-3	330	-333
-1	355	-350
1	332	-333
3	307	-307
5	295	-292
7	244	-251
9	158	-171

H 23 1		
10	125	133
8	187	186
6	225	218
4	261	256
2	271	269
0	281	279
-2	284	283
-4	250	256
-6	198	211
-8	183	195
-10	138	153
H 22 1		
-11	76	-80
-10	41	-33
-9	107	-107
-8	41	-31
-7	140	-132
-5	160	-158
-3	167	-163
-1	213	-209
1	169	-166
3	176	-174
5	174	-169
7	114	-115
9	101	-90
11	66	-75
H 21 1		
11	37	-43
9	50	-47
7	61	-53
6	51	42
5	58	-46
4	49	55
1	46	-43
0	74	65
-2	56	60
-3	45	52
-6	49	45
-7	56	54
-9	56	53
-11	46	49
H 20 1		
-11	97	99
-10	42	-43
-9	116	113
-8	52	-55
-7	135	127
-5	208	206
-3	205	201
-1	199	188
1	222	214
3	233	231
4	45	36
5	154	146
6	62	57
7	133	132
8	49	41
9	144	139
10	69	62
11	69	74
12	45	42
H 19 1		
12	117	-123
11	46	-44
10	215	-212
8	231	-224
6	267	-258
4	385	-378
2	332	-333
0	390	-390
-2	372	-370
-4	314	-313
-6	321	-329
-8	212	-222
-10	169	-183
-12	150	-158
H 18 1		
-13	166	174
-11	208	207
-9	245	241
-7	392	397
-6	48	-55
-5	384	380
-3	421	407
-1	576	567
0	47	-50
1	440	432
3	435	424
4	60	64
5	480	468

7	297	288
9	274	266
10	51	40
11	225	236
13	124	131
H 17 1		
12	219	-221
10	310	-301
8	326	-309
6	518	-510
4	584	-575
3	44	-40
2	543	-540
0	680	-676
-2	694	-680
-4	478	-483
-6	472	-491
-8	416	-431
-10	228	-244
-12	208	-225
H 16 1		
-13	172	174
-12	47	40
-11	172	164
-9	295	282
-8	46	48
-7	376	379
-6	41	35
-5	330	339
-3	474	482
-1	520	522
1	468	472
3	423	425
5	430	431
6	60	-60
7	339	334
9	230	221
10	52	-44
11	224	229
12	44	-42
13	134	139
H 15 1		
14	54	-51
12	114	-112
10	124	-119
8	144	-139
7	50	48
6	205	-203
4	233	-230
2	237	-235
0	240	-242
-2	272	-281
-4	199	-210
-6	155	-162
-8	188	-195
-9	50	-55
-10	105	-107
-12	72	-79
-14	80	-87
H 14 1		
-14	54	57
-12	41	40
-10	86	86
-9	60	53
-8	85	84
-7	100	96
-5	82	74
-4	80	83
-3	90	96
-2	54	54
-1	201	207
1	54	69
3	113	109
5	141	138
6	73	-70
8	77	-86
9	47	36
12	62	-65
H 13 1		
14	78	85
13	100	83
12	95	94
11	108	82
10	139	130
9	121	100
8	266	257
7	152	138
6	233	234
5	97	101
4	236	234

2	523	526
1	101	105
0	310	309
-2	286	296
-3	106	-112
-4	424	443
-6	212	222
-7	93	-92
-8	176	183
-9	131	-123
-10	177	182
-11	100	-85
-12	102	115
-13	82	-66
-14	51	64
-15	72	-69
H 12 1		
-15	111	-122
-13	176	-175
-11	310	-291
-9	370	-367
-8	41	33
-7	385	-394
-5	642	-662
-3	727	-757
-2	70	74
-1	583	-595
0	52	-53
1	845	-841
3	774	-769
5	464	-458
7	495	-478
9	404	-380
11	231	-219
13	175	-176
15	123	-131
H 11 1		
14	179	180
12	231	218
10	366	335
8	467	440
6	468	453
5	82	75
4	671	657
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-13	267	-256
-11	373	-364
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-7	679	-689
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-5	812	-847
-3	871	-905
-2	33	-48
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15	157	-163
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7	107	-103
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Table 5. Continued.

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Table 5. Continued.

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8	159	140	-7	125	126	-3	441	-446		H 11 3		2	205	-202	0	1473	1467	2	147 146
7	457	457	-6	47	30	-1	335	-391	14	160	-162	1	48	-52	-2	1042	1125	0	169 166
6	103	103	-5	154	147	1	454	-457	12	253	-235				-4	791	821	-2	165 167
5	842	834	-3	181	174	2	48	44	10	284	-262	0	209	-212	-6	866	869	-4	145 153
4	273	275	-1	151	155	3	421	-422	9	58	-64	-1	107	-108	-8	592	598	-6	122 134
3	1278	1223	1	180	172	4	59	60	8	427	-395	-3	46	-45	-10	371	369		
2	104	113	3	195	183	5	349	-346	6	517	-494	-4	240	-256	-12	344	333		H 25 4
1	598	614	5	119	114	7	278	-272	4	519	-514	-5	91	-92	-14	234	234		
0	55	50	7	132	126	8	65	44	3	56	-58	-6	97	-90	-16	121	131		
-1	1206	1323	9	98	100	9	268	-259	2	635	-640	-7	88	-90				-8	39 -30
-2	65	-56				11	169	-168	0	679	-684	-9	60	-55		H 2 3		-7	54 -51
-3	1232	1262		H 21 3		13	104	-115	-2	625	-662	-11	111	-107	-15	162	-163	-5	64 -58
-5	580	593	11	34	37				-4	486	-514	-11	46	-58	-13	298	-290	-3	55 -53
-6	116	-112	9	37	42		H 15 3		-6	431	-505	-13	59	-61	-12	79	-76	-1	88 -80
-7	604	614	7	43	37	12	78	72	-8	401	-412				-11	357	-343	1	64 -63
-8	130	-143	5	62	47	11	54	-42	-10	270	-277		H 6 3		-10	64	-74	3	69 -76
-9	515	514	3	63	-52	10	136	120	-12	227	-238	-16	50	67	-9	515	-510	7	33 -41
-10	91	-71	-2	61	-53	8	170	159	-14	166	-181	-15	52	-61	-11	65	-71		
-11	498	484	-3	40	-38	6	169	169				-14	61	79					
-12	105	-86	-5	43	-51	4	182	181											
-13	234	226	-9	53	-49														

Table 5. Continued.

H 24 4

8	40	-41
4	60	-61
2	58	-51
-2	47	-49
-4	54	-50
-7	39	39
-9	32	30

H 23 4

-9	97	102
-7	147	143
-6	48	-42
-5	155	151
-3	168	163
-1	206	196
1	163	149
3	185	178
4	47	44
5	165	164
7	93	92
9	108	119

H 22 4

10	154	-169
8	163	-159
6	248	-237
4	317	-299
2	275	-262
0	335	-322
-2	346	-336
-4	257	-252
-6	265	-266
-8	219	-229
-9	37	16
-10	132	-149

H 21 4

-11	133	144
-9	232	224
-7	318	302
-5	278	265
-3	362	349
-1	401	386
1	338	327
3	331	316
5	329	318
7	244	235
9	180	179

H 20 4

10	169	-169
8	215	-207
6	284	-271
4	332	-318
2	349	-335
0	342	-330
-2	405	-388
-4	318	-310
-6	253	-249
-8	278	-282
-10	164	-174

H 19 4

-11	116	114
-10	47	46
-9	226	214
-7	226	217
-5	236	230
-4	60	59
-3	338	332
-1	312	309
1	270	265
3	312	305
5	254	243
7	190	181
8	41	-26
9	162	158
11	115	118

H 18 4

12	35	-34
11	36	37
10	67	-66
7	68	67
6	55	-56
5	46	43
4	132	-135
2	52	-55
0	80	-84
-2	133	-125
-3	42	-36
-4	76	-77
-6	54	-61
-8	85	-77
-9	71	-64
-10	70	-66

H 17 4

-13	40	-45
-12	35	34
-11	59	-54
-10	54	53
-9	65	-63
-8	55	54
-7	70	-63
-5	116	-109
-3	122	-123
-2	65	63
-1	44	-44
1	147	-144
3	118	-114
7	100	-99
9	60	-59
10	43	-33

H 16 4

13	32	28
12	82	87
11	65	57
10	148	135
9	67	50
8	223	207
6	172	162
5	63	63
4	238	231
2	314	308
0	239	231
-2	240	232
-3	54	-49
-4	280	280
-5	47	-38
-6	200	201
-7	62	-66
-8	156	159
-9	58	-59
-10	149	152
-12	104	114
-13	45	-46

H 15 4

-13	165	-174
-11	248	-241
-9	298	-294
-7	377	-384
-5	476	-485
-3	505	-502
-1	564	-562
1	520	-518
3	527	-518
4	77	-79
5	438	-426
6	47	-63
7	325	-308
9	315	-299
10	69	-67
11	194	-189
12	46	-43
13	127	-129

H 14 4

12	184	181
10	310	294
8	334	316
6	438	427
4	566	566
2	515	513
1	62	-75
0	647	651
-2	624	629
-4	484	497
-6	506	518
-8	393	397
-10	287	285
-12	234	241
-14	160	173

H 13 4

-13	188	-189
-11	208	-196
-9	284	-281
-7	408	-414
-5	354	-367
-3	453	-466
-1	579	-581
0	45	32
1	462	-462
3	454	-446
5	476	-462
7	331	-314
9	281	-262
11	234	-232
13	132	-135

H 12 4

14	85	79
12	148	145
10	224	210
8	263	242
6	375	356
4	452	448
3	37	42
2	488	488
1	44	43
0	472	483
-2	577	602
-3	63	64
-4	422	440
-5	73	74
-6	337	350
-7	41	38
-8	384	367
-10	208	208
-11	60	58
-12	155	159
-14	133	147

H 11 4

-15	54	-55
-14	53	-61
-13	68	-65
-12	74	-75
-10	94	-98
-9	164	-151
-8	75	-79
-7	135	-135
-6	56	-56
-5	72	-62
-4	82	-87
-3	253	-270
-1	171	-168
0	40	47
1	98	-105
2	61	71
3	217	-217
4	108	106
5	132	-134
6	128	126
7	89	-81
8	125	119
9	95	-85
10	67	78
11	85	-78
12	84	86
14	55	62

H 10 4

14	46	-48
13	56	-53
12	50	-55
10	64	-50
8	163	-143
7	68	-67
6	203	-199
4	118	-113
2	292	-300
0	317	-324
-2	163	-169
-3	75	76
-4	256	-270
-5	52	52
-6	246	-254
-8	114	-102
-9	92	87
-10	127	-122
-11	44	50
-12	118	-112
-15	44	45

H 9 4

-15	62	71
-13	124	118
-11	197	195
-10	57	-79
-9	188	183
-8	72	-82
-7	203	203
-5	351	367
-4	82	-83
-3	354	370
-2	96	-97
-1	203	215
1	501	506
3	362	356
5	200	189
7	348	324
9	201	198
11	152	128
13	129	130

H 8 4

14	166	-164
12	217	-207
11	82	-92
10	298	-274
9	92	-99
8	509	-474
7	93	-105
6	517	-491
5	165	-162
4	584	-561
3	74	-75
2	576	-540
1	119	-120
0	736	-747
-1	52	-51
-2	642	-683
-4	774	-828
-6	536	-565
-7	44	59
-8	398	-403
-9	52	69
-10	375	-372
-12	266	-271
-14	155	-159

H 7 4

-15	168	172
-13	280	264
-11	434	413
-9	504	492
-7	629	636
-5	890	930
-3	915	967
-1	943	999
1	1117	1103
2	120	-112
3	995	962
5	713	687
7	619	585
8	63	-96
9	481	450
11	297	278
13	219	215
15	141	147

H 6 4

14	167	-163
12	224	-207
10	324	-299
8	398	-374
7	78	86
6	483	-466
4	617	-587
3	53	60
2	600	-587
1	87	91
0	778	-800
-2	576	-619
-4	513	-544
-6	543	-562
-8	340	-343
-10	308	-298
-12	259	-251
-14	165	-162
-16	107	-111

H 5 4

-15	97	110
-13	190	177
-11	245	237
-9	293	293
-7	463	468
-6	84	84
-5	520	548
-4	54	59
-3	522	553
-2	107	113
-1	767	826
0	67	62
1	685	662
2	106	99
3	563	548
4	93	87
5	560	542
7	362	349
9	289	275
11	225	203
13	120	132
15	83	94

H 4 4

15	49	72
13	72	79
12	92	-68
11	94	115
10	119	-113
9	121	134
8	145	-135
7	131	141
6	217	-217
5	201	200
4	297	-299
3	96	95
2	354	-349
1	96	97
0	333	-357
-1	36	39
-2	418	-451
-3	34	-28
-4	299	-315
-5	114	-116
-6	243	-247
-7	115	-119
-8	253	-246
-9	64	-81
-10	139	-130
-11	133	-136
-12	105	-96
-13	52	-87
-14	77	-80

H 3 4

-16	44	52
-13	84	-83
-12	61	93
-11	187	-182
-10	64	93
-9	156	-155
-8	68	73
-7	279	-279
-6	96	97
-5	461	-470
-4	80	81
-3	269	-280
-2	19	14
-1	367	-363
2	54	-55
3	299	-299
4	73	-77
5	320	-314
6	108	-104
7	216	-217
8	114	-102
9	147	-139
10	85	-77
11	62	-72
12	59	-69

H 2 4

14	117	129
12	161	157
10	201	193
8	321	315
6	396	391
5	128	-131
4	345	394
3	55	-53
2	558	557
1	83	-79
0	699	721
-1	95	-106
-2	385	407
-3	107	-114
-4	492	504
-5	75	-73
-6	481	484
-7	227	227
-9	49	-65
-10	259	251
-12	217	207
-14	79	101
-16	79	92

H 1 4

-15	139	-138
-13	220	-207
-11	364	-351
-10	96	80
-9	372	-366
-8	102	82
-7	443	-452
-5	772	-782
-4	44	46
-3	758	-791
-1	602	-647
0	73	-73
2	188	-197
3	771	-772
4	100	-104
5	499	-496
6	137	-121
7	574	-561
8	199	-175
9	387	-373
10	48	-70
11	255	-241
12	52	-73
13	221	-215
14	43	-61
15	138	-141

H 0 4

14	193	206
12	296	276
10	380	364
8	682	661
6	768	766
4	868	861
2	1615	1574
-4	1362	1375
-6	926	916
-8	651	631
-10	588	556
-12	425	390
-14	224	217
-16	147	174

H 27 5

4	54	59
2	78	71
0	97	96
-2	73	72
-4	72	77

H 26 5

-5	159	-161
-3	145	-141
-1	170	-163
1	178	-178
3	128	-136
5	121	-128

H 25 5

6	172	178
4	193	193
2	240	226
0	262	249
-2	224	218
-4	206	207
-6	214	218

H 24 5

-7	237	-227
-5	253	-238
-3	250	-234
-1	301	-285
1	281	-263
3	237	-235
5	211	-218
7	177	-180

H 23 5

8	124	128
6	185	184
4	197	193
2	206	196
0	260	246
-2	237	224
-4	195	185
-6	195	199
-8	155	167

H 22 5

-9	97	-90
-7	139	-120
-5	138	-125
-3	138	-132
-1	166	-153
1	176	-165
3	107	-107
5	133	-129
7	107	-114
9	61	-63

H 20 5

-11	73	77
-10	56	-42
-9	109	98
-7	146	126
-5	133	125
-3	182	160
-1	192	179
1	154	138
3	144	132
5	173	161
6	55	46
7	82	82
8	58	40
9	68	73

H 19 5

10	129	-135
8	156	-147
6	266	-250
4	252	-234
2	280	-260
0	334	-306
-2	294	-272
-4	300	-276
-6	240	-233
-8	200	-197
-10	154	-164
-12	123	-126

H 18 5

-11	204	197
-9	244	220
-7	294	269
-5	385	364
-3	369	340
-1	402	366
1	448	417
3	347	317
5	335	309
7	306	290
9	181	180
10	49	22

H 17 5

12	149	-161
10	178	-180
8	300	-277
6	370	-348
4	397	-367
2	478	-449
0	544	-505
-2	453	-428
-4	447	-424
-6	444	-426
-8	289	-278
-10	250	-242
-12	197	-209

H 16 5

-13	146	145
-11	209	189
-9	185	173
-8	58	47
-7	332	315
-5	344	336
-3	300	290
-1	438	415
1	377	360
3	324	311
5	316	299
6	60	-39
7	263	251
8	67	-55
9	193	184
11	138	139

H 15 5

12	84	-83
10	94	-92
9	66	37
8	120	-111
6	198	-185
4	195	-181
2	154	-142
0	270	-262
-2	214	-205
-3	67	-55
-4	116	-114
-6	219	-213
-7	76	-54
-8	142	-133
-10	71	-65
-12	111	-111

H 14 5

-14	41	52
-13	48	40
-12	64	59
-8	88	87
-7	70	90
-6	69	67
-5	57	67
-2	71	54
-1	111	111
1	116	108
5	85	77
7	73	51

H 13 5

12	62	63
11	63	72
10	132	134
9	77	81
8	147	145
7	58	82
6	130	124
5	59	77
4	302	298
3	81	97
2	238	237
1	58	47
0	196	200
-2	325	332
-4	218	232
-5	166	176
-7	66	-74
-8	173	177
-10	128	147
-12	75	83
-14	47	64

H 12 5

-13	152	-151
-11	215	-217
-9	313	-313
-4	56	38
-2	355	-365
-6	98	44
-5	365	-383
-3	511	-531
-1	523	-540
1	397	-412
3	476	-483
5	417	-415
7	262	-253
9	247	-251
11	179	-186
13	105	-109

H 11 5

14	111	124
12	183	191
10	271	268
8	304	290
6	435	408
4	481	475
2	497	501

Table 5. Continued.

0	504	521	1	283	280	H	1	5	H	19	6	H	12	6	H	7	6	H	2	6
-2	501	536	2	90	100	14	58	-71	9	112	-121	-14	84	-91	13	162	-167	-14	152	-137
-4	470	502	3	387	375	12	95	-94	7	167	-174	-12	136	-137	11	228	-240	-12	157	-150
-5	46	-32	4	201	184	11	78	89	5	158	-161	-10	248	-242	9	311	-296	-10	161	-152
-6	350	372	5	191	187	10	138	-132	3	224	-217	-9	55	-36	7	472	-435	-8	333	-322
-8	344	353	6	127	111	9	109	109	1	276	-275	-8	220	-217	6	79	86	-7	63	62
-10	280	288	7	180	166	8	175	-163	-1	207	-207	-7	65	-70	5	595	-550	-6	303	-305
-12	194	200				7	119	121	-3	231	-228	-6	290	-297	3	643	-609	-5	96	94
-14	134	148				6	191	-191	-5	259	-258	-5	69	-59	1	709	-705	-4	262	-268
			8	150	129	5	90	103	-6	52	-54	-4	411	-430	0	62	62	-3	78	78
H	10	5	9	184	187	4	169	-171	-7	159	-157	-2	315	-327	-1	756	-798	-2	483	-521
-15	130	-146	10	211	137	3	121	126	-9	138	-141	-1	58	-57	-3	636	-682	-1	78	83
-13	202	-205	11	101	105	2	326	-331				0	399	-399	-5	572	-596	0	393	-399
-11	305	-308	13	57	67	1	69	78	-11	136	-146	1	57	-55	-7	571	-572	1	68	65
-9	399	-403				0	199	-211				2	399	-395	-9	417	-409	-2	484	-521
-7	432	-458	H	5	5	-2	149	-162	H	18	6	4	298	-293	-11	304	-293	3	111	105
-5	602	-641	14	118	-124	-4	306	-314	-10	61	55	6	272	-260	-13	247	-242	4	416	-401
-3	660	-701	12	155	-162	-5	65	-65	-6	84	76	8	212	-214	-15	144	-167	6	304	-293
-1	641	-667	10	308	-297	-6	112	-120	-4	108	95	10	136	-150				8	208	-197
0	96	-100	8	400	-379	-7	65	-61	-2	76	59	12	97	-97				10	181	-185
1	768	-775	6	405	-399	-8	133	-129	0	76	60							12	150	-143
2	55	-47	4	758	-738	-9	106	-108	2	120	123	H	11	6				14	69	-80
3	609	-607	2	767	-750	-10	143	-146	4	54	49	13	56	35	H	6	6			
5	570	-535	1	39	30	-11	103	-82	8	77	80	12	60	-59	-14	167	159	H	1	6
6	72	-76	0	643	-672	-12	79	-76				10	89	-82	-12	206	196	13	154	157
7	474	-443	-1	32	36	-15	85	-69	H	17	6	9	77	68	-10	247	240	11	254	248
9	317	-304	-2	849	-930				11	46	42	8	63	-67	-8	369	371	9	284	266
11	245	-253	-4	678	-738	H	0	5	7	52	56	7	122	109	-6	368	379	7	387	364
13	157	-166	-6	503	-526	-10	93	95	5	97	94	6	92	-89	-4	385	411	6	141	150
			-7	66	72	-8	74	71	1	95	90	5	65	61	-2	548	593	5	554	547
H	9	5	-8	494	-500	-6	57	61	-1	110	105	4	96	-89	-1	39	-49	4	78	79
14	103	110	-10	391	-391	-4	131	125	-3	55	51	3	94	98	0	465	473	3	477	469
12	177	179	-12	226	-218	-2	107	112	-5	85	76	2	85	-79	2	512	488	2	77	80
10	222	216	-14	178	-179	2	51	41	-7	69	68	1	211	214	4	505	471	1	583	582
8	335	315				4	115	111	-9	54	58	-1	58	57	5	69	-72	0	89	94
7	106	-101	H	4	5				-12	41	-43	-3	106	110	6	390	364	-1	626	725
6	441	424	-15	171	174	H	27	6				-5	200	204	8	332	313	-2	30	40
5	52	-60	-13	202	191	-1	145	163	H	16	6	-6	75	78	10	240	232	-3	494	516
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-13	97	-89				-2	49	27	9	202	201	-2	233	250	-6	69	-62	6	644	-629
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H	6	5	4	132	-135				3	415	405	-1	68	64						
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																		-9	90	-87

Table 5. Continued.

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7	179	-186
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3	268	-277
1	294	-281
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-3	302	-288
-5	266	-257
-7	253	-245
-9	193	-192
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2	336	329
4	305	308
6	241	254
8	182	192
10	141	163
H 16 7		
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9	140	-151
7	167	-190
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3	294	-286
1	257	-250
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-5	215	-206
-7	222	-225
-9	225	-213
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8	103	104
10	86	92
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H 13 7		
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6	133	-142
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8	123	-135
9	74	-63
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11	64	-45
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H 12 7		
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6	304	-292
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6	303	-295
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12	74	81
H 0 7		
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H 24 8		
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H 23 8		
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1	106	116
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H 22 8		
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H 20 8		
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H 16 8		
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8	74	63
H 10 8		
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-2	107	-103
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-6	83	-59
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H 9 8		
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H 8 8		
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H 6 8		
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-6	288	-281
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H 4 8		
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6	90	-91
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2	117	-110
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-12	74	-71
H 3 8		
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3	158	-162
5	65	-67
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-5	59	-58
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-7	65	-65
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-14	72	79
H 1 8		
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4	92	-96
5	321	-315
7	237	-263
9	217	-249
H 0 8		
10	193	227
8	298	305
6	324	323
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-2	600	613
-4	583	563
-6	473	444
-8	416	388
-10	377	348
-12	228	215
-14	128	160

were therefore removed from the data set before the final refinement. The remaining 3706 were not corrected for multiple reflection effects.

Refinement with anisotropic temperature factors was performed with constant inter-layer scale factors, the isotropic extinction parameter still being allowed to vary. In the final refinement, which yielded $R = 0.044$, weights calculated with Cruickshank's formula [7] $w = (a + F_o + cF_o^2 + dF_o^3)^{-1}$, where $a = 25.0$, $c = 0.01$ and $d = 0.00025$, were used. The corresponding weight analysis is given in Table 3. The final structure parameters are listed in Table 4 and the observed and calculated structure factors are compared in Table 5. Atomic scattering factors due to Cromer and Waber [8] for Te, and to Doyle and Turner [9] for K^+ and O were used in the refinement. The Te and K^+ scattering factors were corrected for anomalous dispersion according to Cromer.[10] The least squares programmes used were BLOCK [11] (block-diagonal approximation) and LINUS [12] (full matrix).

A difference electron density summation computed from the final parameters did not reveal the positions of the hydrogen atoms, which is to be expected since tellurium is present. Although residuals as high as 3 $e/Å^3$ appeared in the vicinity of the Te positions, there were no other regions of unexplained electron density. The Fourier summation was carried out with the FFT (Fast Fourier Transform) [13,14] programs designed by Ten Eyck,[15] the summation of all 3706 reflections at 41 000 points taking only 30 sec central unit time on an IBM 360/65 computer.

DISCUSSION

The tellurium(VI) atoms in $KTeO_3(OH)$ are octahedrally coordinated by oxygen atoms, the octahedra being connected through edges to form infinite chains parallel to the c axis (*cf.* Fig. 1). This was already shown in 1964 by

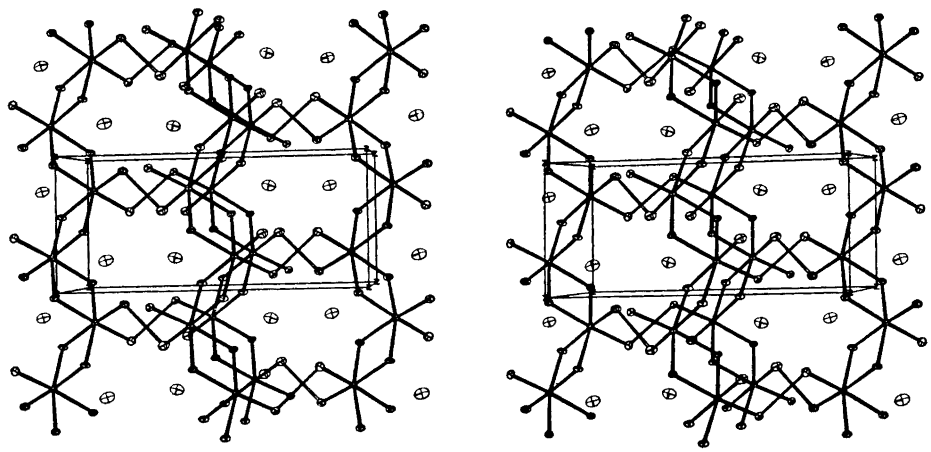

Fig. 1. A stereoscopic view [24] along the a axis showing the $[TeO_3(OH)]_n^{n-}$ chains. The thermal ellipsoids enclose areas with an atomic probability density greater than 50 %.

Lammers,[2] and although he solved the structure in the wrong space group using equatorial data only, his Te – O bond distances do not deviate appreciably from the present values. There are differences, however, in the O – Te – O angles and in the O – O distances (*cf.* Table 6).

Table 6. Tellurium – oxygen coordination distances (Å) and angles (°) in $KTeO_3(OH)$. The values in the last columns have been calculated from the positions given by Lammers.[2] The notation is in accordance with Fig. 2.

Distances			Angles		
$Te-O_1$	1.945(2)	1.96	O_1-Te-O_1'	78.3(1)	79
$Te-O_1'$	1.997(2)	2.01	O_1-Te-O_2	90.0(1)	93
$Te-O_2$	1.994(2)	2.01	O_1-Te-O_2'	164.8(1)	168
$Te-O_2'$	1.947(2)	1.96	O_1-Te-O_3	93.4(1)	96
$Te-O_3$	1.883(3)	1.84	O_1-Te-O_4	97.4(1)	92
$Te-O_4$	1.843(3)	1.84	$O_1'-Te-O_2$	89.0(1)	85
			$O_1'-Te-O_2'$	92.3(1)	93
O_1-O_1'	2.488(4)	2.52	$O_1'-Te-O_3$	171.1(1)	172
O_1-O_2	2.785(3)	2.88	$O_1'-Te-O_4$	90.4(1)	90
O_1-O_3	2.787(4)	2.83	O_2-Te-O_2'	77.9(1)	79
O_1-O_4	2.847(3)	2.74	O_2-Te-O_3	87.6(1)	90
$O_1'-O_2$	2.797(3)	2.73	O_2-Te-O_4	172.3(1)	172
$O_1'-O_2'$	2.843(3)	2.88	$O_2'-Te-O_3$	95.1(1)	92
$O_1'-O_4$	2.726(3)	2.73	$O_2'-Te-O_4$	94.5(1)	96
O_2-O_2'	2.477(4)	2.52	O_3-Te-O_4	94.1(1)	95
O_2-O_3	2.685(4)	2.73			
$O_2'-O_3$	2.828(4)	2.74	Hydrogen bond		
$O_2'-O_4$	2.785(3)	2.83	$O_3\cdots O_4$	2.480(4)	2.62
O_3-O_4	2.782(4)	2.73			

The $[TeO_3(OH)]_n^{n-}$ chains are held together by electrostatic interaction with the potassium ions and through very strong hydrogen bonds between O_3 and O_4. The $O_3\cdots O_4$ distance is 2.480 Å, and is thus much shorter than the

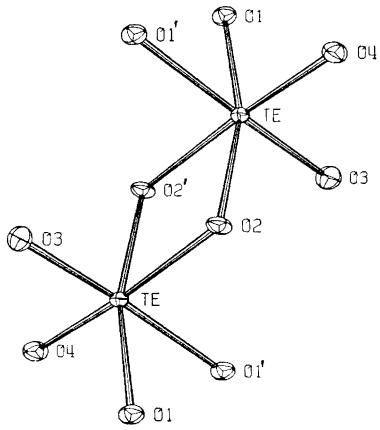

Fig. 2. The oxygen coordination of two symmetry related tellurium atoms. The notation used in Table 6 is indicated.

value of 2.62 Å given by Lammers. The potassium ion has six oxygen contacts at normal distances ranging from 2.654 Å to 2.983 Å (*cf.* Table 7), with a mean value of 2.782 Å.

Table 7. Potassium – oxygen distances (Å) below 3.7 Å. The values in the last column have been calculated from the positions given by Lammers.

$K-O_3$	2.654(3)	2.66
$K-O_4$	2.661(3)	2.66
$K-O_2$	2.762(2)	2.78
$K-O_4$	2.804(3)	2.86
$K-O_1$	2.828(2)	2.78
$K-O_3$	2.983(3)	2.86
$(K-O_1$	3.434(2)	3.65)

The presence of the heavy Te atom in the structure prevented the location of the positions of the hydrogen atoms in the final electron density maps. With an O···O distance as short as 2.480 Å, the question, however, arises as to the character of the hydrogen bond. As pointed out by Blinc and Hadži [16] no definite predictions can be made from the magnitude of the O···O separation alone. In this case, however, the significant difference between the $Te-O_3$ (1.883 Å) and the $Te-O_4$ (1.843 Å) bonds indicates that the hydrogen atom ought to be attached to O_3, and thus that an antisymmetric hydrogen bond is present. An argument against this might be that the $Te-O_3$ distance is shorter than the Te – OH distances in other tellurates, which usually range from 1.93 Å to 2.03 Å, and is even shorter than those in $Te(OH)_6$, where the average Te – OH bond distance is 1.916 Å.[17] However, a comparable situation occurs in $KH_5(PO_4)_2$ [18] in which a very short hydrogen bond of 2.405 Å is accompanied by P – O distances of 1.512 Å and 1.516 Å, both significantly shorter than the ordinary P – OH distances of 1.549 – 1.560 Å and just slightly longer than the P – O distances of 1.490 Å and 1.502 Å. A recent neutron diffraction investigation [19] has shown that the hydrogen bond is slightly antisymmetric, with O – H = 1.174 Å and H···O = 1.252 Å. It is interesting to note that in both $KTeO_3(OH)$ and $KH_5(PO_4)_2$, both Me – O distances involved in the short hydrogen bond are shorter than the average value between an ordinary

Table 8. Bridging dimensions in tellurates containing octahedra sharing edges.

	Te – O (Å)	O – Te – O (°)
$K_4[Te_2O_6(OH)_4](H_2O)_{7.3}$ [21]	1.985(9)	77.6(4)
	2.029(10)	
$Na_2K_4[Te_2O_8(OH)_2](H_2O)_{14}$ [22]	2 × 2.026(21)	78.8(6)
$Na_{0.5}K_{3.5}[Te_2O_6(OH)_4](H_2O)_6$ [23]	1.992(14)	77.5(8)
	2.027(16)	
$KTeO_3(OH)$	1.945(2)	78.3(1)
	1.997(2)	
	1.947(2)	77.9(1)
	1.994(2)	

Me – OH and a "keto" Me – O bond. In $KH_5(PO_4)_2$ this average value is 1.526 Å, and in $KTeO_3(OH)$ it ought to lie in the range 1.88 – 1.94 Å, *i.e.* between the corresponding mean values calculated for $KTeO(OH)_5.H_2O$ [20] and $K_4[Te_2O_6(OH)_4](H_2O)_{7.3}$.[21]

The dimensions of the Te – O – Te bridges in $KTeO_3(OH)$ are in close agreement with those in other tellurates containing the same type of double bridges. There are small differences in the Te – O distances, but the large deviations of the O – Te – O angles from 90° are of almost exactly the same magnitude in all the compounds compared in Table 8.

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