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X-ray Diffraction Refinement of the Calcium Tungstate Structure

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The crystal structure of $CaWO_4$ (scheelite) has been refined with single-crystal x-ray diffraction data. For the tetragonal cell $\underline{a} = 5.243 \pm 0.002$, $\underline{c} = 11.376 \pm 0.003$ Å. Oxygen coordinates 0.1504, 0.0085, 0.2111 correspond to Ca—O distances 2.44 and 2.48 Å and W—O distances 1.78 Å.

INTRODUCTION

We became interested in the crystal structure of calcium tungstate (scheelite) because we wished to compare it with the closely-related structure of europium tungstate which we recently determined.[1] The scheelite structure was investigated by Sillén and Nylander[2] who reviewed earlier work and determined oxygen coordinates from considerations of shape and size. They confirmed this structure with a limited amount of x-ray data. We have refined this structure with more precise x-ray diffraction data to obtain oxygen coordinates which agree with those of Sillén and Nylander within the accuracy which they claimed. A recent study by neutron diffraction[3] is in excellent agreement with our results for both coordinates and thermal parameters.

EXPERIMENTAL

We used a large triply-pulled single crystal of synthetic $CaWO_4$ which was grown by Dr. Kurt Nassau at the Bell Telephone Laboratory. A trapezoidal fragment was chipped from the large boule; it was roughly a parallelopiped of dimensions 0.015 × 0.035 × 0.11 mm. It was mounted on a goniometer head with the long dimension (the [110] direction) as the axis of rotation. Measurements were made with a General Electric XRD-5 goniostat, scintillation counter, and Mo x-ray tube (λ = 0.70926 Å for $K\alpha_1$). Intensities were measured for 828 independent reflections permitted by the space group ($2\theta < 100^\circ$), 163 of which were recorded as zero. Each was counted for 20 sec. The most intense reflection, (112), was 1000 counts/sec. The smallest increment recorded by the scaler was 0.5 counts/sec. Background at the larger angles was 0.5 to 1.0 counts/sec.

We estimate the linear absorption coefficient as 405 cm^{-1} for MoKα radiation. Absorption corrections were calculated by a numerical integration for a rectangular prism which approximated the shape of the crystal. These factors ranged from 1.8 to 2.7 and were checked by the angular variation of intensities with phi for reflections with chi equal 90°. The intensities were corrected by an empirical function for the alpha-doublet separation, which was complete for the higher angles. A correction for extinction was made with an empirical factor 2500/(2500 - I), where I is the observed intensity in counts/sec. This correction had an insignificant effect on most of the intensities, but increased the strongest by a factor 1.7.

Atomic scattering factors for Ca^{+2} and neutral O and W were taken from International Tables,[4] Table 3.3.1A. The values for O were increased slightly below $\sin\theta/\lambda = 0.2$ to approximate a charge state of $-\frac{1}{2}$. Values for the dispersion correction $\Delta f'$ were taken from Table 3.3.2C.[4] The correction $\Delta f''$ was taken as 0.4 for Ca and 7.5 for W.

We minimized the function $\sum w(|F_o|-|F_c|)^2/\sum wF_o^2$ with a least-squares program[5] which we modified to include the effect of the imaginary dispersion correction in the calculation of $|F_c|$. Each reflection was given unit weight. Atoms were given anisotropic temperature factors of the form $\exp(-\beta_{11}h^2 -\beta_{22}k^2 -\beta_{33}\ell^2 -2\beta_{12}hk -2\beta_{13}h\ell -2\beta_{23}k\ell)$, with suitable constraints for the Ca and W atoms. Refinement was continued until no parameter changed in the sixth decimal place. $R = \sum||F_o|-|F_c||/\sum|F_o|$ was reduced to 0.061. The final observed and calculated structure factors are listed in Table I.

RESULTS

The space group is $I4_1/a$. For the body-centered cell we find, with the synthetic $CaWO_4$:

$a = 5.243 \pm 0.002$, $c = 11.376 \pm 0.003$ Å.

These values are in good agreement with those of Swanson et al.[6] who report 5.242 and 11.372 from powder data. We compared powder photographs (CuKα radiation) of our synthetic $CaWO_4$ and of a sample of natural scheelite. No difference in cell dimensions could be detected, also in agreement with Swanson et al.[6]

There are two distinct ways in which the axial system may be oriented with respect to the structure; one is changed to the other by interchange of the a and b axes (and reversal of c if one wishes to preserve the handedness of the axes). The orientation of a particular specimen which corresponds to our oxygen coordinates may be determined by comparison of the intensities: (121) weaker than (211), (123) stronger than (213).. In our calculations the correct orientation was determined by trial and error.

The parameters and standard deviations determined by least squares are listed in Table II together with the neutron-diffraction results of Kay, Frazer and Almodovar.[3] The coordinates agree more closely than the claimed accuracy, and the thermal parameters differ at most by little more than the sum of the two standard deviations. This concordance is gratifying evidence of the accuracy of both methods. These results are stated with the origin at the center of symmetry. If the origin is placed at a tungsten atom, our coordinates for oxygen can be chosen as 0.2435, 0.1504, 0.0861 to conform with the setting used by Sillén and Nylander.[2]

The structure is shown in Fig. 1. The interatomic distances less than 3.7 Å are listed in Table III. Calcium has 8 oxygen neighbors at an average distance of 2.46 Å. The WO_4 group is nearly regular tetrahedral with O—W—O angles 107.5° (4 times) and 113.4° (2 times). These distortions from a regular tetrahedron are not much outside our limits of error, but are confirmed very precisely by the neutron diffraction results. The

W—O bond distance 1.784 Å becomes 1.789 Å when corrected for thermal motion with the assumption that O rides on W. The fact that the tetrahedron is not regular is consistent with the much larger distortions observed in $Eu_2(WO_4)_3$ in which the environment is less symmetrical.[1] In the latter structure, the nearest-neighbor W—O distances average 1.74 and 1.78 Å for two kinds of W atoms.

We thank Prof. A. Pabst for giving us some crystals of scheelite and Dr. M. P. Klein for giving us the synthetic crystal.

References

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[5]P. K. Gantzel, R. A. Sparks and K. N. Trueblood, private communication.

[6]H. E. Swanson, N. T. Gilfrich and M. I. Cook, Natl. Bur. Standards U. S. Circ. No. 539, 6, 23 (1956).

Table I. Observed structure factor magnitudes (FOB) and calculated structure factors (FCA).

(table to be reproduced photographically)

H,K= 0, 0
L FCO FCA
4 240-252
8 210 193
12 206-196
16 120 110
20 84 -86
24 74 69

H,K= 0, 1
L FOO FCA
1 175-154
3 163-151
5 110 100
7 105 79
9 117 -99
11 95 -89
13 82 74
15 71 65
17 49 -48
19 46 -40
21 44 40
23 36 33

H,K= 0, 2
L FCO FCA
0 215-240
2 31 -25
4 255 293
6 0 -2
8 215-210
10 10 9
12 149 143
14 0 7
16 135-126
18 0 1
20 85 86
22 0 -2
24 54 -55

H,K= 0, 3
L FOB FCA
1 112 104
3 106 82
5 135-117
7 121-108
9 83 74
11 78 69
13 68 -64
15 62 -54
17 62 55
19 43 46
21 30 -30
23 26 -26

H,K= 0, 4
L FOB FCA
0 204 209
2 34 -32
4 192-194
6 0 -3
8 175 171
10 16 16
12 137-138
14 0 14
16 102 103
18 0 3
20 77 -76
22 0 -5

H,K= 0, 5
L FOB FCA
1 96 -92
3 90 -84
5 82 81
7 77 77
9 74 -69
11 69 -65
13 61 57
15 45 46
17 40 -41
19 36 -37
21 38 31

H,K= 0, 6
L FOB FCA
0 157-157
2 21 -17
4 154 151
6 0 -2
8 137-133
10 0 11
12 114 108
14 15 10
16 84 -85
18 0 2
20 72 64

H,K= 0, 7
L FOB FCA
1 70 65
3 76 73
5 60 -56
7 52 -51
9 65 60
11 52 50
13 42 -42
15 46 -43
17 32 32
19 33 26

H,K= 0, 8
L FOB FCA
0 126 121
2 0 -3
4 106-105
6 0 -0
8 94 95
10 0 2
12 91 -88
14 0 2
16 72 65

H,K= 0, 9
L FOB FCA
1 48 -49
3 46 -43
5 49 47
7 46 46
9 24 -37
11 36 -37
13 27 35

H,K= 0,10
L FOB FCA
0 71 -72
2 0 1
4 83 81
6 0 0
8 80 -72
10 0 -1

H,K= 0,11
L FOB FCA
1 37 32
3 37 34
5 45 -35

H,K= 1, 1
L FOB FCA
2 293-313
4 64 54
6 235 250
8 38 34
10 194-186
12 11 5
14 145 141
16 0 -10
18 106-102
20 16 -10
22 79 73
24 0 -3

H,K= 1, 2
L FOB FCA
1 90 -83
3 141 135
5 140 120
7 124-107
9 103 -91
11 72 65
13 66 58
15 67 -65
17 64 -58
19 42 45
21 30 36
23 26 -26

H,K= 1, 3
L FOB FCA
2 215 206
4 15 10
6 224-225
8 9 8
10 152 156
12 0 2
14 124-125
16 0 -3
18 103 102
20 0 -3
22 66 -63

H,K= 1, 4
L FOB FCA
1 121 106
3 97 -89
5 90 -79
7 87 79
9 82 77
11 82 -75
13 68 -66
15 51 51
17 35 40
19 34 -37
21 32 -33

H,K= 1, 5
L FOB FCA
2 182-193
4 0 -1
6 143 139
8 0 -1
10 149-148
12 0 0
14 117 110
16 0 1
18 71 -71
20 0 0

H,K= 1, 6
L FCO FCA
1 85 -82
3 69 67
5 76 72
7 73 -68
9 57 -57
11 59 59
13 57 52
15 36 -39
17 39 -38
19 33 34

H,K= 1, 7
L FCB FCA
2 129 127
4 0 4
6 132-130
8 0 4
10 101 99
12 0 1
14 85 -83
16 0 -2
18 74 69

H,K= 1, 8
L FCB FCA
1 54 50
3 64 -60
5 56 -53
7 49 49
9 51 50
11 37 -38
13 35 -35
15 42 39
17 38 31

H,K= 1, 9
L FCB FCA
2 99 -93
4 0 7
6 87 87
8 0 7
10 80 -76
12 0 1
14 62 63

H,K= 1,10
L FOB FCA
1 42 -40
3 38 39
5 39 38
7 31 -37
9 37 -34
11 32 32

H,K= 1,11
L FOB FCA
2 71 65
4 0 4

H,K= 2, 1
L FOB FCA
1 162-156
3 87 -80
5 134 106
7 122 105
9 79 -68
11 96 -87
13 87 80
15 57 49
17 56 -51
19 52 -47
21 24 30
23 36 32

H,K= 2, 2
L FCB FCA
0 249-284
2 0 6
4 223 211
6 8 1
8 193-186
10 0 -2
12 198 158
14 0 -2
16 111-109
18 0 -1
20 80 81
22 0 0

H,K= 2, 3
L FOB FCA
1 98 80
3 140 123
5 93 -80
7 83 -75
9 108 99
11 74 68
13 55 -55
15 67 -64
17 44 44
19 29 34
21 41 -40
23 32 -28

H,K= 2, 4
L FOB FCA
0 201 202
2 25 22
4 102-103
6 10 3
8 161 160
10 16 -11
12 133-134
14 0 -10
16 98 98
18 0 -3
20 70 -72
22 0 3

H,K= 2, 5
L FOB FCA
1 101 -95
3 81 -76
5 78 75
7 73 71
9 64 -63
11 64 -67
13 65 59
15 46 43
17 34 -38
19 32 -34
21 27 28

H,K= 2, 6
L FOB FCA
0 150-148
2 15 12
4 148 144
6 0 2
8 128-128
10 0 -7
12 109 103
14 0 -8
16 80 -82
18 0 -3
20 63 62

H,K= 2, 7
L FOB FCA
1 57 56
3 61 61
5 71 -68
7 67 -64
9 49 49
11 40 41
13 40 -38
15 39 -38
17 38 38

H,K= 2, 8
L FOB FCA
0 102 102
2 0 1
4 109-108
6 0 1
8 103 96
10 0 -0
12 76 -75
14 0 -1
16 73 66

H,K= 2, 9
L FOB FCA
1 52 -49
3 44 -45
5 42 40
7 40 38
9 34 -39
11 48 -39
13 37 35

H,K= 2,10
L FOB FCA
0 92 -83
2 0 -2
4 75 70
6 0 0
8 69 -65
10 0 1

H,K= 2,11
L FOB FCA
1 32 32
3 41 35

H,K= 3, 1
L FOB FCA
2 228-235
4 8 -9
6 183 180
8 10 -7
10 174-175
12 0 -1
14 135-131
16 14 2
18 92 -88
20 0 3
22 77 71

H,K= 3, 2
L FOB FCA
1 141-125
3 110 92
5 83 67
7 79 -70
9 94 -84
11 97 87
13 84 73
15 56 -51
17 40 -37
19 33 39
21 30 36
23 40 -34

H,K= 3, 3
L FOB FCA
2 203 200
4 0 9
6 181-177
8 0 7
10 156 153
12 0 1
14 122-116
16 0 -3
18 74 86
20 0 -3
22 73 -64

H,K= 3, 4
L FOB FCA
1 85 78
3 90 -83
5 106 -97
7 95 89
9 70 65
11 59 -55
13 51 -52
15 50 48
17 49 48
19 40 -41
21 33 -28

H,K= 3, 5
L FOB FCA
2 159-155
4 11 10
6 162 156
8 12 9
10 121-110
12 0 1
14 99 97
16 0 -5
18 84 -79
20 0 -4

H,K= 3, 6
L FOB FCA
1 70 -65
3 85 78
5 61 60
7 57 -55
9 67 -65
11 52 49
13 44 41
15 41 -46
17 31 -34
19 27 27

H,K= 3, 7
L FOB FCA
2 123 121
4 0 1
6 115-109
8 0 1
10 96 97
12 0 -1
14 83 -78
16 0 -1
18 60 60

H,K= 3, 8
L FOB FCA
1 61 56
3 41 -43
5 49 -51
7 57 50
9 36 37
11 41 -42
13 40 -40
15 26 28

H,K= 3, 9
L FOB FCA
2 69 -88
4 0 -4
6 81 77
8 0 -4
10 70 -73
12 0 -1

H,K= 3,10
L FOB FCA
1 50 -39
3 40 38
5 31 33
7 32 -32
9 32 -34

H,K= 4, 1
L FOB FCA
1 97 -84
3 121-110
5 93 81
7 83 76
9 93 -89
11 69 -67
13 55 55
15 61 59
17 45 -44
19 34 -34
21 31 37

H,K= 4, 2
L FOB FCA
0 195-206
2 12 13
4 180 181
6 0 0
8 162-159
10 0 -7
12 141 136
14 0 -6
16 103 -96
18 0 -1
20 75 72
22 0 3

H,K= 4, 3
L FOB FCA
1 100 95
3 76 71
5 97 -91
7 97 -87
9 64 59
11 70 65
13 61 -60
15 41 -41
17 46 44
19 43 41
21 32 -27

H,K= 4, 4
L FOB FCA
0 153 148
2 0 -4
4 172-169
6 0 -1
8 146 145
10 0 2
12 106-102
14 0 2
16 95 94
18 0 1
20 66 -67

H,K= 4, 5
L FOB FCA
1 70 -65
3 81 -75
5 76 72
7 67 66
9 59 -60
11 48 -48
13 46 43
15 43 45
17 36 -39
19 33 -32

H,K= 4, 6
L FOB FCA
0 145-140
2 0 -2
4 122 119
6 0 -1
8 115-107
10 0 1
12 102 99
14 0 1
16 70 -70
18 0 1

H,K= 4, 7
L FOB FCA
1 70 62
3 61 56
5 42 -45
7 46 -43
9 57 49
11 48 48
13 46 -42
15 37 -34
17 26 26

H,K= 4, 8
L FOB FCA
0 104 97
2 0 4
4 89 -92
6 0 0
8 86 84
10 0 -3
12 79 -71
14 0 -3

H,K= 4, 9
L FOB FCA
1 41 -38
3 47 -42
5 42 42
7 43 40
9 36 -35
11 32 -30

H,K= 4,10
L FOB FCA
0 76 -66
2 0 4
4 73 68
6 0 0

H,K= 5, 1
L FOB FCA
2 165-169
4 0 -4
6 180 182
8 0 -4
10 122-126
12 0 -1
14 104 103
16 0 1
18 89 -89
20 0 2

H,K= 5, 2
L FOB FCA
1 75 -71
3 97 91
5 88 84
7 80 -76
9 75 -71
11 54 52
13 48 46
15 52 -52
17 45 -43
19 40 35
21 32 31

H,K= 5, 3
L FOB FCA
2 163 163
4 15 -14
6 141-142
8 18 -13
10 128 125
12 0 -2
14 102-100
16 0 6
18 71 73
20 0 6

H,K= 5, 4
L FOB FCA
1 77 77
3 70 -70
5 65 -65
7 62 61
9 65 58
11 63 -57
13 56 -49
15 42 40
17 36 35
19 26 -31

H,K= 5, 5
L FOB FCA
2 137-132
4 12 -13
6 125 120
8 13 -12
10 110-105
12 0 -2
14 86 84
16 0 6
18 77 -64

H,K= 5, 6
L FOB FCA
1 68 -63
3 46 51
5 51 54
7 59 -53
9 47 -43
11 45 46
13 41 44
15 31 -32
17 33 -30

H,K= 5, 7
L FOB FCA
2 104 103
4 0 -4
6 96 -90
8 0 -4
10 86 84
12 0 -0
14 74 -68

H,K= 5, 8
L FOB FCA
1 36 40
3 45 -48
5 40 -42
7 41 39
9 43 41
11 32 -33
13 26 -28

H,K= 5, 9
L FOB FCA
2 77 -71
4 0 1
6 89 76
8 0 1
10 60 -58

H,K= 5,10
L FOB FCA
1 32 -32
3 32 33

H,K= 6, 1
L FOB FCA
1 73 -69
3 72 -73
5 83 80
7 75 75
9 59 -59
11 43 -49
13 47 46
15 40 44
17 39 -42
19 30 -36

H,K= 6, 2
L FOB FCA
0 139-141
2 0 -8
4 148 148
6 0 -1
8 129-129
10 0 5
12 100 99
14 0 5
16 87 -85
18 0 1
20 67 61

H,K= 6, 3
L FOB FCA
1 81 75
3 76 70
5 57 -57
7 55 -54
9 62 59
11 56 56
13 46 -48
15 46 -41
17 26 32
19 27 27

H,K= 6, 4
L FOB FCA
0 141 145
2 0 1
4 118-116
6 0 0
8 111 106
10 0 -1
12 104-102
14 0 -1
16 72 67
18 0 -0

H,K= 6, 5
L FOB FCA
1 56 -57
3 66 -60
5 54 53
7 55 50
9 58 -51
11 43 -43
13 45 38
15 38 37
17 27 -30

H,K= 6, 6
L FOB FCA
0 96 -95
2 0 -1
4 103 109
6 0 -0
8 102 -93
10 0 0
12 70 70
14 0 1
16 74 -65

H,K= 6, 7
L FOB FCA
1 47 46
3 44 41
5 45 -48
7 40 -46
9 38 34
11 31 35
13 32 -33

H,K= 6, 8
L FOB FCA
0 88 80
2 0 -5
4 84 -76
6 0 -1
8 72 70
10 0 4

H,K= 6, 9
L FOB FCA
1 37 -35
3 45 -36
5 32 33
7 36 31

H,K= 7, 1
L FOB FCA
2 133-135
4 0 -1
6 117 114
8 0 -1
10 107-107
12 0 1
14 88 86
16 0 1
18 67 -62

H,K= 7, 2
L FOB FCA
1 71 -69
3 52 52
5 67 63
7 68 -61
9 44 -44
11 54 50
13 47 47
15 26 -32
17 33 -34

H,K= 7, 3
L FOB FCA
2 122 121
4 0 6
6 116-110
8 0 6
10 101 96
12 0 2
14 81 -78
16 0 -2
18 66 60

H,K= 7, 4
L FOB FCA
1 55 55
3 59 -59
5 50 -48
7 43 46
9 51 51
11 42 -42
13 37 -38
15 39 37
17 33 28

H,K= 7, 5
L FOB FCA
2 100-100
4 0 7
6 97 97
8 0 7
10 84 -81
12 0 2
14 77 66

H,K= 7, 6
L FOB FCA
3 45 -41
5 47 48
7 46 -45
9 39 -39
11 35 32
13 41 29

H,K= 7, 7
L FOB FCA
2 85 79
4 0 2
6 84 -77
8 0 2
10 72 64

H,K= 7, 8
L FOB FCA
1 69 -63
3 56 -53
5 32 -32
7 37 31

H,K= 8, 1
L FOB FCA
1 69 -63
3 56 -53
5 45 46
7 44 44
9 44 -47
11 50 -49
13 39 42
15 33 32
17 33 -26

H,K= 8, 2
L FOB FCA
0 110-108
2 0 -2
4 112 104
6 95 -95
8 0 -0
10 0 1
12 74 79
14 0 1
16 64 -63

H,K= 8, 3
L FOB FCA
1 48 45
3 55 51
5 59 -54
7 57 -50
9 47 43
11 31 35
13 33 -32
15 34 -33

H,K= 8, 4
L FOB FCA
0 92 91
2 0 -5
4 95 -96
6 0 -0
8 86 85
10 0 4
12 77 -68
14 0 3

H,K= 8, 5
L FOB FCA
1 46 -48
3 40 -39
5 38 43
7 36 41
9 33 -34
11 40 -37
13 45 35

H,K= 8, 6
L FOB FCA
0 84 -82
2 0 -2
4 76 75
6 0 0
8 78 -69
10 0 2

H,K= 8, 7
L FOB FCA
1 38 35
3 49 40
5 37 -32
7 30 -30

H,K= 8, 8
L FOB FCA
0 76 64

H,K= 9, 1
L FOB FCA
2 97 -94
4 0 5
6 87 86
8 0 5
10 79 -77
12 0 0
14 60 63

H,K= 9, 2
L FOB FCA
1 42 -42
3 35 31
5 40 42
7 41 -39
9 47 -44
11 32 34
13 27 29

H,K= 9, 3
L FOB FCA
2 83 83
4 0 -0
6 82 -86
8 0 -0
10 70 68
12 0 -1

H,K= 9, 4
L FOB FCA
1 42 41
3 38 -39
5 50 -42
7 41 40
9 33 33
11 34 -32

H,K= 9, 5
L FOB FCA
2 80 -77
4 0 -1
6 72 65
8 0 -1
10 72 -64

H,K= 9, 6
L FOB FCA
1 43 -39
3 34 34
5 40 31
7 35 -30

H,K=10, 1
L FOB FCA
1 34 -39
3 39 -38
5 39 41
7 41 39
9 38 -32
11 33 -30

H,K=10, 2
L FOB FCA
0 90 -79
2 0 4
4 78 73
6 0 1
8 71 -66
10 0 -3

H,K=10, 3
L FOB FCA
1 41 39
3 36 38
5 37 -33
7 38 -32
9 38 34

H,K=10, 4
L FOB FCA
0 78 69
2 0 5
4 69 -66
6 0 1

H,K=10, 5
L FOB FCA
1 38 -33
3 38 -34

H,K=11, 1
L FOB FCA
2 72 -64
4 0 -3

H,K=11, 2
L FOB FCA
1 46 -36
3 32 32

Table II. Parameters and standard deviations from least squares.[a]

Parameter	This work	Neutron diffraction[b]
Oxygen		
x	0.1504 ± 0.0013	0.1511 ± 0.0006
y	0.0085 ± 0.0014	0.0087 ± 0.0005
z	0.2111 ± 0.0006	0.2111 ± 0.0001
β_{11}	0.0100 ± 0.0016	0.0057 ± 0.0012
β_{22}	0.0115 ± 0.0016	0.0073 ± 0.0014
β_{33}	0.0016 ± 0.0003	0.0016 ± 0.0003
β_{12}	0.0016 ± 0.0013	0.0014 ± 0.0007
β_{13}	0.0004 ± 0.0006	0.0004 ± 0.0002
β_{23}	0.0008 ± 0.0006	0.0005 ± 0.0002
Calcium		
β_{11}	0.0071 ± 0.0004	0.0051 ± 0.0022
β_{33}	0.0011 ± 0.0001	0.0019 ± 0.0006
Tungsten		
β_{11}	0.0036 ± 0.0001	0.0038 ± 0.0022
β_{33}	0.00095 ± 0.00003	0.00038 ± 0.00053

[a]Origin at center of symmetry. Ca at $\pm(0, \frac{1}{4}, \frac{5}{8}) + \underset{\sim}{I}$. W at $\pm(0, \frac{1}{4}, \frac{1}{8}) + \underset{\sim}{I}$. O at $\pm(x, y, z;\ -x, \frac{1}{2} - y, z;\ \frac{3}{4} - y, \frac{1}{4} + x, \frac{1}{4} + z;\ \frac{1}{4} + y, \frac{1}{4} - x, \frac{1}{4} + z) + \underset{\sim}{I}$. $\underset{\sim}{I} = (0, 0, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

[b]Ref. 3.

Table III. Interatomic distances in $CaWO_4$.

Atom	Neighbors	Distance,[a] Å
Ca	4 O	2.44
	4 O	2.48
W	4 O[b]	1.78
	4 O	2.91
O	W	1.78
	W	2.91
	Ca	2.44
	Ca	2.48
	2 O[b]	2.88
	O[b]	2.98
	2 O	2.77
	O	2.88
	2 O	2.94
	O	3.04
	O	3.14

[a]Standard deviations 0.01 Å for Ca—O and W—O distances and 0.02 Å for O—O distances.

[b]Neighbor in same WO_4 group.

(figure caption)

Fig. 1. Crystal structure of $CaWO_4$. The number on each atom is its y coordinate X 100.

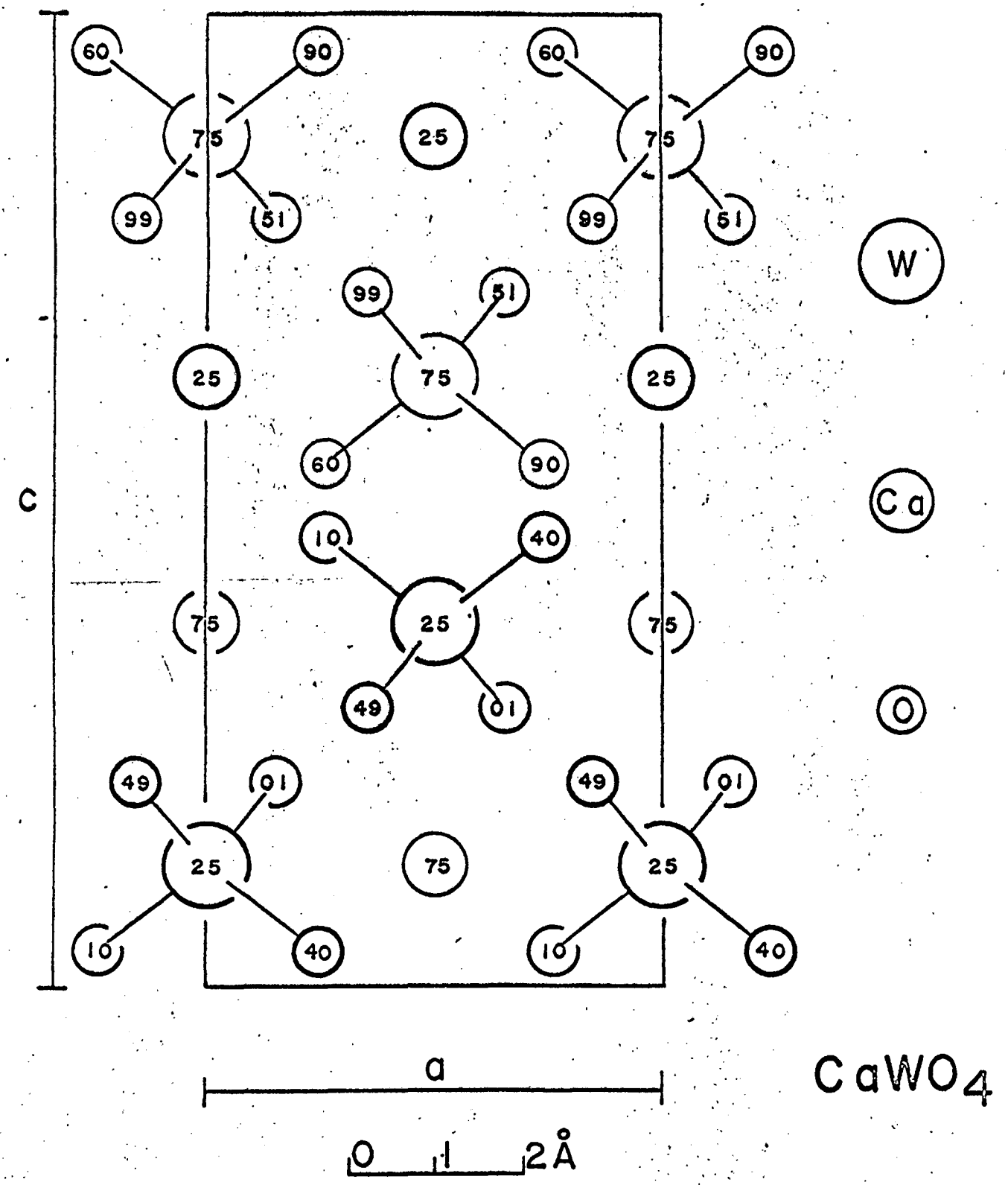

Fig. 1.