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CRYSTAL STRUCTURE OF CERIUM MAGNESIUM NITRATE HYDRATE

A. Zalkin, J. D. Forrester, and D. H. Templeton

July, 1963

Crystal Structure of Cerium Magnesium Nitrate Hydrate*

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According to single-crystal x-ray diffraction data, crystals of $Ce_2Mg_3(NO_3)_{12}.24H_2O$ are rhombohedral, space group $R\bar{3}$. The hexagonal cell with a = 11.004 ± 0.006, c = 34.592 ± 0.012 Å contains 3 formula units. Atomic parameters were refined by least squares, and interatomic distances were corrected for thermal motion. The average N—O bond distance in nitrate is 1.26 Å. The Ce atoms, on the 3-fold axis at z = ± 0.2497, are each surrounded by 12 oxygen atoms at an average distance of 2.64 Å. These oxygen atoms, belonging to 6 nitrate ions, are at the corners of a somewhat irregular icosahedron. The Mg atoms are of two kinds, located respectively at the origin and on the 3-fold axis at z = ± 0.4279. Each Mg atom is surrounded by 6 water molecules with the

oxygen atoms at the corners of an octahedron with an average Mg—O distance of 2.07 Å. One-fourth of the water molecules are not coordinated to cations. Evidence for the hydrogen atom positions from the diffraction data indicates that 6 of the 8 independent hydrogen atoms are involved in normal hydrogen bonds.

INTRODUCTION

Cerium magnesium nitrate hydrate is a typical member of the extensive series of double nitrates of generic formula $T_2D_3(NO_3)_{12}\cdot 24H_2O$, where T is a trivalent cation (e. g., Bi or an ion of the 4f group) and D is a divalent cation (e. g., Mg or an ion of the 3d group). Double nitrate crystals have been used extensively in experiments involving magnetic cooling, nuclear alignment, or paramagnetic resonance.[1] Large crystals are easy to grow, and the cations are at sites of favorable symmetry and sufficiently far enough apart for these purposes. Considerable information pertaining to the structure has been obtained from the resonance experiments and by x-ray diffraction, but the complete structure has not been determined previously. Lack of this information has hindered the interpretation of paramagnetic resonance studies.[2] We investigated this structure because of the wide interest in these substances and because of our interest in hydrogen bonding in salt hydrates.

We have obtained x-ray diffraction data for a single crystal of cerium magnesium nitrate hydrate of sufficient accuracy to locate all of the atoms including hydrogen. These data showed immediately a discrepancy

with previous reports of the symmetry. The other double nitrates are expected to have structures very similar to that reported here for the cerium magnesium salt.

EXPERIMENTAL

An aqueous solution of cerous nitrate and magnesium nitrate in the correct proportions was allowed to evaporate, and single crystals of the double nitrate grew readily in the form of thick hexagonal plates. X-ray photographs obtained with the Weissenberg technique and copper radiation established the diffraction symmetry of the crystal. A single crystal of approximate dimensions 0.09 × 0.20 × 0.15 mm was used for collecting intensity data. Intensities were measured with a General Electric XRD-5 goniostat equipped with a scintillation counter and a pulse-height discriminator; MoKα radiation was used throughout. The unit cell dimensions are based on $\lambda = 0.70926$ Å for $MoK\alpha_1$.

The 2381 independent reflections permitted by the space group in the sphere with $\sin\theta/\lambda$ less than 0.705 ($2\theta < 60^\circ$) were measured with counting times of 20 sec each. Of these, 561 were assigned zero intensity. Reflections with odd ℓ are systematically weaker than those of even ℓ, especially at large diffraction angles. Zero intensity was assigned to only one reflection with even ℓ. Among the 478 odd-ℓ reflections for $50^\circ < 2\theta < 60^\circ$, 327 were recorded as zero and 119 as 0.5 counts/sec (the smallest increment recorded by the scaler). None was stronger than 2 counts/sec. In the same angular range, only 2 of the 457 even-ℓ reflections were recorded as 2 counts/sec or less.

Such a large block of zero or nearly-zero intensities was considered undesirable in the least-squares calculations, and we arbitrarily assigned zero weight to the 788 reflections which were measured as less than 2.5 counts/sec and for which 2θ exceeded 40°. Unit weight was assigned to each of the remaining 1593 reflections, including 109 recorded as zero.

No corrections were made for either absorption or extinction, but the crystal was dipped in liquid nitrogen in an endeavor to reduce the latter. With $\mu = 22.7$ cm^{-1} for Mo radiation, μr is 0.23 or less. Thus absorption, though small, is not negligible and is a limiting factor in the accuracy of the intensity data.

Calculations were made with IBM-709 and 7090 computers using a full-matrix least-squares program written by P. K. Gantzell, R. A. Sparks and K. N. Trueblood, with minor changes, and Fourier and distance programs written by Zalkin. We minimized $\sum w(|F_o|-|F_c|)^2/\sum wF_o^2$.

Atomic scattering factors were taken as the values given by Ibers[3] for Mg^{+2} and neutral N, O and H, and the values given by Thomas and Umeda[4] for Ce^{+3}. Dispersion is unimportant for these atoms with Mo radiation,[5] and no dispersion correction was made.

UNIT CELL AND SPACE GROUP

The primitive cell containing one formula unit $Ce_2Mg_3(NO_3)_{12}\cdot 24H_2O$ is rhombohedral with dimensions:

$$a(r) = 13.165 \pm 0.006 \text{ Å}, \qquad \alpha(r) = 49.37^\circ.$$

The corresponding hexagonal cell containing three formula units has dimensions:

$$a = 11.004 \pm 0.006 \text{ Å}, \qquad c = 34.592 \pm 0.012 \text{ Å}.$$

These results are compared in Table I with some previous measurements. In the often-quoted but unpublished work of Powell[6] the weak odd-ℓ reflections were overlooked, and the c dimension was assigned half of its correct value. Except for this error, which was recognized by Culvahouse, Unruh and Sapp[7] and by Swanson, et al.,[8] the various results are in reasonable agreement.

From our x-ray data the density is calculated as 2.10 g cm^{-3}. A measurement by a flotation method gave 2.08 g cm^{-3}.

Reflections are absent unless $h-k-\ell = 3n$, showing that the primitive lattice is rhombohedral. No further systematic absences were observed. A careful examination of the Weissenberg photographs and of the data collected with the goniostat confirmed the 3-fold symmetry but showed that there are no vertical mirror planes, in direct contradiction to the result of Culvahouse, Unruh and Sapp.[7] Thus the Laue group is $\bar{3}$ (C_{3i}). These facts leave the choice of space group between the centrosymmetric $R\bar{3}$ (C_{3i}^2) and the noncentric R3 (C_3^4). Crystal morphology[9] suggests a center of symmetry; while the point group is listed as $\bar{3}m$ ("trigonal skalenoëdrisch") the observed faces are equally consistent with point group $\bar{3}$ because of the absence of general forms. On the other hand, the observed faces would correspond to equal development of four non-equivalent pairs of forms if the point group were 3. The success of our structure determination confirms $\bar{3}$ as the point group and $R\bar{3}$ as the space group.

DETERMINATION OF THE STRUCTURE

A three-dimensional Patterson function was calculated from the observed intensities after correction for Lorentz and polarization effects.

The hexagonal unit cell contains 6 Ce atoms which are identical according to magnetic evidence.[10] The only 6-fold set available is

$$6(c): \quad \pm(0,0,z) + (0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}).$$

We selected z = 0.25 because any other value is inconsistent with the weak reflections with ℓ odd. There is also a huge Patterson peak at $0,0,\frac{1}{2}$, but it turned out that much of this peak is due to many pairs of light atoms.

Paramagnetic resonance data[11] indicate that there are two different types of divalent ions. The 9 Mg atoms must be assigned to a 3-fold set and a 6-fold set. Without loss of generality, the 3-fold set is chosen as

$$\text{Mg(1) in 3(a):} \quad (0,0,0) + (0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}).$$

The Patterson function contains peaks corresponding to Ce-Mg interactions with Mg(2) in 6(c) with z = 0.43 (or 0.07). The choice 0.07 places Mg atoms unreasonably close together and does not fit possible Mg-Mg interactions in the Patterson function. The parameter 0.43 places pairs of Mg atoms nearly equidistant from each other and from neighboring Ce atoms along the 3-fold axis, and is confirmed by the subsequent refinement.

All other atoms are in general positions

$$18(f): \quad \pm(x,y,z;\ -y,x-y,z;\ y-x,-x,z) + (0,0,0;\ \tfrac{1}{3},\tfrac{2}{3},\tfrac{2}{3};\ \tfrac{2}{3},\tfrac{1}{3},\tfrac{1}{3}).$$

The structure requires 2 sets of N atoms, 10 sets of oxygen atoms, and 8 sets of H atoms.

From the Patterson function we chose coordinates for 5 sets of oxygen atoms. The parameters of the 8 sets of atoms so far located were refined by least squares using 617 low-angle reflections. Three

cycles reduced $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$ to 0.40. With phases determined by these 8 atoms, an electron density function showed the locations of the 2 sets of N atoms and the remaining 5 sets of O atoms.

With these 15 atoms, 617 reflections and isotropic temperature factors of the form $\exp(-B\lambda^{-2}\sin^2\theta)$ least-squares refinement resulted in R = 0.086 after three cycles. Further refinement with all the data (1593 terms selected as described earlier) after 3 cycles gave R = 0.064. These 15 atoms were given anisotropic temperature factors of the form $\exp(-\beta_{11}h^2 -\beta_{22}k^2 -\beta_{33}\ell^2 -2\beta_{12}hk -2\beta_{13}h\ell -2\beta_{23}k\ell)$. The atoms on the 3-fold axis (i. e., Ce and Mg) had their parameters constrained so that

$$\beta_{11} = \beta_{22} = 2\beta_{12}, \text{ and } \beta_{13} = \beta_{23} = 0.$$

As a result of 3 cycles, R fell to 0.040.

An electron density difference function, with all atoms except H subtracted out, was calculated using the results of the anisotropic refinement. From this difference function, 7 of the 8 hydrogen positions (all in general sets 18(f)) were unambiguously determined. The eighth proved to be more difficult to determine as the difference function was confused in the appropriate region, leaving a choice of two locations. The more likely of these had much too high a peak height, possibly due to an incorrect thermal description of the oxygen atoms, but it was more reasonable on the basis of bond geometry.

Three cycles of least squares refinement were calculated with all 23 atoms, 15 of which had anisotropic temperature factors and the remaining 8 (the H atoms) isotropic temperature factors. With 149 independent parameters and using all the data (weighted as described earlier) the final R was 0.036. The observed and calculated structure factors from

this last refinement are compared in Table II. Coordinates of atoms are listed in Table III, and thermal parameters are given in Tables IV and V. Standard deviations of the parameters of the heavy atoms were calculated assuming that the discrepancies in the structure factors represent random errors and with neglect of the hydrogen parameters. Limitations of our computer programs did not permit us to estimate the standard deviations of the hydrogen parameters by the method of least squares. From the results for O—H bond distances, we estimate that the standard deviations of H coordinates correspond to about 0.2 Å.

DESCRIPTION OF THE STRUCTURE

A section through the structure parallel to $\underline{c}$ and $[\bar{1}10]$ is shown in Fig. 1. The structure consists of Ce atoms surrounded by nitrate ions, and Mg atoms surrounded by water. One set of water molecules (W_4) is not closely associated with any cation, but participates in the hydrogen bonding which connects the nitrate ions and water.

Much of the structure nearly repeats with a translation of $\underline{c}/2$. Only the Mg and H atoms diverge substantially from this pattern. The Ce positions conform to this false translation within 0.01 Å. This repetition explains the general weakness of the odd-ℓ reflections.

The symmetry of the Ce environment (the site symmetry) is 3 (C_3), but it can be considered to be more symmetrical if for some purpose only some of the neighbors are important. If one considers only Ce neighbors, the site symmetry is 3m (C_{3v}) and very nearly $\bar{3}$m (D_{3d}). The nearest Ce neighbors are 3 at 8.56 Å and 3 at 8.59 Å. If one considers also the Mg atoms, the site symmetry is still 3m, but deviates drastically from $\bar{3}$m. The nearest Mg neighbors (Fig. 2) are 1 at 6.17 Å,

3 each at 6.36, 6.98 and 8.31 Å, and 1 at 8.64 Å.

The nearest neighbors of the Ce atom are oxygen atoms of nitrate ions (Fig. 3) arranged at the 12 corners of an irregular icosahedron. Their positions conform closely to inversion symmetry so that the site symmetry is approximately $\bar{3}$ (C_{3i}) if only the nitrate ions are considered. The coordination by nitrate ions was predicted by Bleaney *et al.*[12] from paramagnetic resonance data, but with a different number and arrangement of neighbors. From spectroscopic data Judd[13] deduced icosahedral symmetry of these neighbors in qualitative agreement with our result. According to Hellwege and Hellwege[14] spectroscopic data show the symmetry of the crystal field to be C_{3v}. To make the 12 oxygen atoms conform to vertical mirror planes or to make the icosahedron regular requires that they be moved distances of the order of 0.5 Å. This result may indicate a limitation of the precision with which crystal field effects can be used to determine the symmetry of atomic locations.

The 12-fold coordination of Ce, which may seem higher than normal, is permitted by the fact that two oxygen atoms in the same nitrate ion are closer together than when not bonded to each other. The distances of these neighbors from Ce are nearly equal (Table VI) and average 2.63 Å before correction for thermal motion. If a thermal correction is made on the assumption that O "rides on" Ce, the average distance is 2.64 Å. The accuracy of this assumption is dubious, but in any case the thermal correction is not a large effect.

The N—O bond distances are listed in Table VII. In each of the two independent nitrate ions the oxygen not next to Ce is observed at a shorter distance and with larger thermal motion than the others. For these bonds the assumption that O "rides on" N seems plausible. Correction on this

basis brings the bond lengths more nearly together, but leaves a discrepancy which is of doubtful significance. The average distance 1.26 Å is estimated to be accurate within 0.01 Å including uncertainty in the thermal correction. We do not know of any other more accurate determination of this bond distance in nitrate ion.

There are two distinctly different types of Mg atoms in the structure. The atoms Mg(1) at the origin have site symmetry $\bar{3}$ (C_{3i}). If only Ce and Mg neighbors are considered, the site symmetry is $\bar{3}m$ (D_{3d}). The neighbors (Fig. 4) include 6 Ce at 6.98 Å (at the corners of a trigonal antiprism) and 2 Ce at 8.64 Å. The nearest Mg neighbors are 6 Mg(2) at 7.15 Å.

The atoms Mg(2) have site symmetry 3 (C_3). Considering only Ce and Mg neighbors, this symmetry is 3m (C_{3v}). The neighbors (Fig. 5) include 1 Ce at 6.17 Å and 3 Ce each at 6.36 and 8.31 Å. The nearest Mg neighbors are 1 Mg(2) at 4.99 Å and 3 Mg(1) at 7.15 Å. This arrangement is rather different from that suggested by Culvahouse et al.[7] on the basis of paramagnetic resonance data.

Each kind of Mg has six water neighbors. The oxygen atoms are at the corners of an octahedron which would be regular if bond angles were changed by less than 1° for Mg(1) and by up to 5° for Mg(2). The Mg—O distances (Table VIII) agree closely. Correction for thermal motion with the assumption that O "rides on" Mg changes them only a small amount. The average corrected distance 2.07 Å agrees closely with the similar distances observed[15,16] in $Mg(NH_4)_2(SO_4)_2.6H_2O$ and $MgSO_4.6H_2O$. That the divalent ions are octahedrally hydrated was already established by paramagnetic resonance,[17] and nuclear magnetic resonance experiments[18] showed that water was distant from the cerium sites.

We may formulate this substance as

$$(Mg(H_2O)_6)_3(Ce(NO_3)_6)_2 \cdot 6H_2O$$

as a concise indication of the coordination of Mg and Ce and the chemically distinct nature of the fourth set of water molecules.

HYDROGEN BONDING

Hydrogen bonding is extensive in this crystal, but it does not seem to dominate the structure as much as it does in many hydrated salts. Six of the 8 H atoms are involved in normal hydrogen bonds with lengths ranging from 2.78 to 2.98 Å (Table IX). The angles that these bonds make with each other and with the O—Mg vectors are listed in Table X. In each case the angles are appropriate for reasonable orientations of the water molecules with their dipoles away from the Mg atoms.

The accuracy of the hydrogen positions does not justify a detailed listing of the distances and angles to these atoms. The O—H bond distances range from 0.5 to 0.9 Å. The O—H bonds make angles of 8° to 29° with the O—O vectors of the corresponding hydrogen bonds. These results are as good as can be expected if the standard deviations of hydrogen coordinates correspond to 0.2 Å.

For O(W4) no neighbor is at a suitable distance and angle for the second H atom to make a normal hydrogen bond. Two neighbors, O(N22) at 2.98 Å and O(N21) at 3.09 Å, are close enough for weak bonding, but at poor angles. The hydrogen atom H(2W4) is directed within 28° of O(N21) and within 40° of O(N22). This kind of arrangement (Fig. 6) has been called a "bifurcated hydrogen bond". In the present case, the distances suggest that the bonding is weak.

For the second hydrogen of O(W3), the bonding situation is even poorer. The O(W3)-H(2W3) vector is within 29° of another O(W3) at 3.20 Å and within 54° of O(N22) at 3.08 Å. This hydrogen atom was the one most in doubt in the difference function, but its position corresponds to an H—O—H angle of 111° for the water molecule and an H—O—Mg angle of 120°. We conclude that it is not significantly involved in hydrogen bonding.

The hydrogen bonding ties the structure together as follows. Water (W2) is bonded to two oxygen atoms of two different nitrate ions. Water (W3) is bonded through only a single hydrogen bond to the interstitial water (W4). Water (W1) is bonded to a nitrate ion and to water (W4). Water (W4) accepts two hydrogen bonds and makes a third to nitrate. Its "bifurcated bond" involves oxygen atoms of two other nitrate ions. The effect of all these hydrogen bonds is to tie all parts of the structure together.

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*Work done under the auspices of the U. S. Atomic Energy Commission.

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Table I. Cell dimensions and axial ratios of Ce-Mg salt.

a, Å	c, Å	c/a	Reference
11.004	34.592	3.144	This work.
10.88	34.44[a]	3.165[a]	Powell (Ref. 6).
11.030	34.65	3.141	Swanson et al. (Ref. 8).
--	--	3.0756[a]	Groth (Ref. 9).

[a]Value doubled to conform with correct cell.

Table II. Observed structure factor magnitudes (FOB) and calculated structure factors (FCA). An asterisk (*) marks each reflection which was given zero weight.

(Table to be reproduced photographically in three parts.)

H,K= 0, 0
L FOB FCA
3 39 34
6 264-250
9 118 113
12 44 -38
15 10 -15
18 344-346
21 67 62
24 32 -18
27 51 -55
30 15 -7
33 66 66
36 117 122
39 0 1*
42 138-149
45 0 -19*
48 91 104

H,K= 1,-1
L FOB FCA
2 391-363
5 101 94
8 176 176
11 0 1
14 471-474
17 0 -17
20 306 310
23 32 24
26 0 0
29 15 14
32 132 137
35 34 26*
38 114-115
41 26 3*
44 79 83
47 0 -4*

H,K= 1, 0
L FOB FCA
1 58 -51
4 402 368
7 100 94
10 65 -64
13 10 10
16 232 237
19 0 10
22 195-200
25 19 20
28 224 224
31 0 10
34 194-190
37 25 22*
40 138 130
43 19 -13*
46 84 -82

H,K= 1, 1
L FOB FCA
0 353 328
3 51 47
6 225-218
9 12 6
12 480 486
15 15 -19
18 154-157
21 69 68
24 221 230
27 20 -21
30 122-120
33 28 52*
36 135 135
39 32 -6*
42 79 -77
45 0 17*
48 63 65

H,K= 1, 2
L FOB FCA
2 37 22
5 116 107
8 35 -24
11 10 9
14 291-296
17 12 -9
20 168 173
23 41 42
26 196-203
29 0 -8
32 193 193
35 24 9*
38 90 -87
41 0 0*
44 106 99
47 0 2*

H,K= 1, 3
L FOB FCA
1 19 -22
4 175 180
7 95 90
10 368-368
13 43 -43
16 316 319
19 22 24
22 14 -22
25 41 42
28 162 166
31 16 -14*
34 105 -98
37 31 27*
40 149 138
43 20 0*
46 100-110

H,K= 1, 4
L FOB FCA
0 322 329
3 31 -34
6 256-254
9 65 68
12 297 293
15 0 2
18 97-100
21 0 7
24 223 222
27 16 7
30 102 -94
33 46 49
36 79 77
39 0 -11*
42 108-103
45 0 11*

H,K= 1, 5
L FOB FCA
2 131-135
5 96 93
8 149 152
11 43 -42
14 239-239
17 14 23
20 146 148
23 15 15
26 100-105
29 0 -13*
32 120 122
35 26 27*
38 95 -90
41 0 -3*
44 92 88

H,K= 1, 6
L FOB FCA
1 26 -35
4 265 261
7 43 44
10 264-259
13 0 5
16 198 194
19 0 -1
22 167-169
25 0 12*
28 224 214
31 18 10*
34 78 -80
37 28 27*
40 65 68

H,K= 1, 7
L FOB FCA
0 224 220
3 20 16
6 253-253
9 26 22
12 102 102
15 27 -26
18 152-151
21 23 32*
24 191 186
27 25 -8*
30 45 -40
33 27 33*
36 87 84
39 0 -1*

H,K= 1, 8
L FOB FCA
2 158-159
5 31 30
8 32 32
11 16 -11
14 52 -51
17 17 21*
20 158 155
23 0 11*
26 106 -96
29 0 2*
32 91 86
35 0 6*

H,K= 1, 9
L FOB FCA
1 17 -18*
4 103 100
7 65 63
10 68 -64
13 17 -19*
16 157 150
19 18 10*
22 99 -97
25 19 18*
28 99 98
31 0 -12*
34 90 -86

H,K= 1,10
L FOB FCA
0 108 110
3 0 -10*
6 158-155
9 36 27*
12 127 121
15 0 -15*
18 83 -81
21 0 2*
24 80 79
27 0 5*
30 76 -69

H,K= 1,11
L FOB FCA
2 112-120
5 0 1*
8 96 97
11 0 1*
14 71 -65
17 0 14*
20 65 63
23 0 -3*

H,K= 1,12
L FOB FCA
1 0 3*
4 95 97
7 0 15*
10 68 -70
13 0 -3*
16 66 67

H,K= 2,-2
L FOB FCA
1 31 -29
4 428 422
7 67 55
10 400-402
13 20 20
16 356 364
19 24 21
22 215-222
25 0 13
28 217 228
31 16 10
34 134-138
37 30 30*
40 74 74
43 20 -19*
46 92 -90

H,K= 2,-1
L FOB FCA
3 31 29
6 522-504
9 38 28
12 40 46
15 11 -8
18 323-322
21 38 34
24 231 233
27 48 -41
30 121-121
33 40 37
36 146 145
39 32 -16*
42 69 -65
45 0 16*
48 82 85

H,K= 2, 0
L FOB FCA
2 78 -74
5 121 112
8 169 171
11 54 -44
14 94-100
17 53 46
20 154 153
23 42 38
26 154-147
29 21 -16
32 178 182
35 45 37
38 158-154
41 27 -4*
44 101 96
47 0 -6*

H,K= 2, 1
L FOB FCA
1 44 -43
4 80 -73
7 82 78
10 322-325
13 41 -43
16 269 276
19 25 28
22 104-108
25 42 42
28 184 184
31 0 1
34 223-222
37 0 1*
40 143 143
43 20 -20*
46 68 -65

H,K= 2, 2
L FOB FCA
0 86 89
3 30 -30
6 624-618
9 72 73
12 435 441
15 44 -50
18 114-125
21 60 57
24 136 141
27 0 -5
30 143-148
33 17 14*
36 83 80
39 26 -21*
42 48 -46
45 0 18*

H,K= 2, 3
L FOB FCA
2 240-248
5 43 47
8 239 240
11 33 -38
14 59 -63
17 71 76
20 93 100
23 0 4
26 155-159
29 0 10
32 74 73
35 0 17*
38 101 -97
41 28 -24*
44 130 131

H,K= 2, 4
L FOB FCA
1 57 -56
4 207 208
7 110 114
10 357-364
13 58 -61
16 199 205
19 0 17
22 159-160
25 35 35
28 148 144
31 24 -32*
34 94 -96
37 33 26*
40 119 110
43 0 -9*

H,K= 2, 5
L FOB FCA
0 145 150
3 0 6
6 186-184
9 23 26
12 220 216
15 0 -5
18 238-243
21 15 17
24 173 173
27 0 -21*
30 90 -91
33 26 29*
36 108 108
39 20 -6*
42 51 -53

H,K= 2, 6
L FOB FCA
2 57 -62
5 24 25
8 282 281
11 0 11
14 173-172
17 0 -3
20 145 146
23 0 18*
26 110-108
29 26 20*
32 68 68
35 0 1*
38 95 -92
41 21 -1*

H,K= 2, 7
L FOB FCA
1 26 24
4 138 141
7 0 11
10 114-115
13 32 -31
16 113 107
19 29 37*
22 195-191
25 0 -8*
28 116 116
31 0 -6*
34 90 -83
37 0 10*

H,K= 2, 8
L FOB FCA
0 191 190
3 16 -10
6 128-122
9 0 44*
12 86 87
15 24 -26*
18 126-121
21 18 19*
24 114 114
27 19 7*
30 89 -87
33 0 4*

H,K= 2, 9
L FOB FCA
2 95 -95
5 25 13*
8 43 40
11 18 -12*
14 83 -82
17 19 21*
20 112 113
23 0 2*
26 82 -81
29 0 2*

H,K= 2,10
L FOB FCA
1 0 -8*
4 105 101
7 0 17*
10 108-105
13 0 -3*
16 110 113
19 0 8*
22 45 -50
25 0 4*

H,K= 2,11
L FOB FCA
0 154 160
3 0 11*
6 69 -69
9 20 21*
12 73 72
15 0 -14*
18 83 -87
21 0 11*

H,K= 2,12
L FOB FCA
2 66 -69
5 0 -5*
8 59 57

H,K= 3,-3
L FOB FCA
3 72 69
6 193-205
9 63 61
12 652 665
15 0 -8
18 287-293
21 82 83
24 185 192
27 21 -22
30 190-195
33 17 34*
36 30 28
39 19 -27*
42 55 -50
45 0 8*

H,K= 3,-2
L FOB FCA
2 230-237
5 58 57
8 716 717
11 35 35
14 92 -94
17 33 31
20 117 121
23 41 40
26 229-233
29 15 -20
32 132 137
35 0 1*
38 48 -52
41 19 25*
44 102 103
47 0 11*

H,K= 3,-1
L FOB FCA
1 53 -54
4 502 495
7 92 85
10 196-206
13 0 -1
16 287 286
19 43 45
22 341-337
25 0 6
28 244 243
31 0 -13
34 84 -87
37 40 35
40 111 112
43 0 -8*
46 87 -88

H,K= 3, 0
L FOB FCA
0 224 218
3 36 -42
6 32 -36
9 79 71
12 155 164
15 11 -9
18 183-185
21 59 61
24 231 229
27 0 3
30 209-205
33 0 13*
36 155 143
39 19 -9*
42 105-101
45 20 18*

H,K= 3, 1
L FOB FCA
2 261-260
5 0 -13
8 144 147
11 22 -18
14 12 -7
17 58 56
20 280 289
23 0 13
26 159-158
29 0 18
32 134 136
35 17 15*
38 110-119
41 19 -11*
44 101 101

H,K= 3, 2
L FOB FCA
1 15 13
4 275 280
7 101 103
10 261-266
13 68 -71
16 229 233
19 63 61
22 60 -66
25 15 28
28 170 168
31 0 -12*
34 159-160
37 37 30*
40 99 105
43 20 -21*
46 95-100

H,K= 3, 3
L FOB FCA
0 371 370
3 38 -40
6 285-289
9 58 70
12 283 285
15 0 -11
18 75 -83
21 50 53
24 122 114
27 0 -0
30 152-150
33 0 8*
36 74 73
39 19 -17*
42 70 -70

H,K= 3, 4
L FOB FCA
2 183-184
5 18 23
8 218 219
11 0 -3
14 77 -81
17 14 19
20 146 149
23 0 12
26 70 -67
29 0 3*
32 149 145
35 27 22*
38 108-103
41 0 11*

H,K= 3, 5
L FOB FCA
1 36 36
4 236 233
7 0 10
10 184-183
13 0 -0
16 227 228
19 41 46
22 193-196
25 0 -1*
28 114 111
31 18 -1*
34 94 -95
37 20 11*
40 69 71

H,K= 3, 6
L FOB FCA
0 179 176
3 15 18
6 204-206
9 43 46
12 186 188
15 45 -47
18 96 -96
21 56 58
24 138 131
27 0 -14*
30 68 -69
33 0 8*
36 81 77
39 0 5*

H,K= 3, 7
L FOB FCA
2 175-176
5 0 2
8 153 151
11 28 15*
14 38 -34
17 17 6*
20 148 144
23 18 6*
26 86 -88
29 19 22*
32 73 69
35 0 0*

H,K= 3, 8
L FOB FCA
1 0 -0*
4 93 90
7 24 24*
10 97 -92
13 0 -11*
16 164 163
19 19 18*
22 91 -89
25 0 16*
28 88 78
31 0 -1*

H,K= 3, 9
L FOB FCA
0 110 113
3 0 2*
6 102 -97
9 0 9*
12 176 171
15 19 5*
18 115-114
21 20 22*
24 70 68
27 0 -13*

H,K= 3,10
L FOB FCA
2 84 -85
5 19 16*
8 68 61
11 0 -1*
14 87 -79
17 0 -1*
20 75 78
23 0 10*

H,K= 3,11
L FOB FCA
1 0 6*
4 68 81
7 0 -0*
10 46 -49
13 0 4*

H,K= 4,-4
L FOB FCA
2 130-140
5 45 47
8 121 123
11 20 13
14 118-124
17 28 13
20 204 209
23 0 9
26 178-181
29 0 -2
32 140 142
35 18 15*
38 95 -93
41 19 -0*
44 114 113

H,K= 4,-3
L FOB FCA
1 52 53
4 219 226
7 30 27
10 299-304
13 11 -11
16 204 208
19 68 66
22 290-292
25 29 -30
28 197 203
31 16 -3*
34 81 -81
37 31 33*
40 128 131
43 0 -15*
46 75 -82

H,K= 4,-2
L FOB FCA
3 16 15
6 223-224
9 69 65
12 355 355
15 44 -47
18 83 -91
21 94 94
24 225 230
27 26 -32
30 96 -99
33 0 23*
36 142 135
39 19 18*
42 98 -97
45 21 16*

H,K= 4,-1
L FOB FCA
2 632-632
5 22 22
8 391 387
11 0 5
14 76 66
17 30 34
20 111 111
23 14 17
26 124-127
29 0 4
32 80 74
35 17 3*
38 131-133
41 0 -4*
44 134 134

H,K= 4, 0
L FOB FCA
1 0 -5
4 283 284
7 53 55
10 225-222
13 17 -22
16 244 251
19 60 61
22 322-322
25 0 -7
28 167 163
31 29 -20
34 81 -82
37 18 32*
40 158 154
43 0 -9*
46 59 -54

H,K= 4, 1
L FOB FCA
0 304 306
3 56 -50
6 436-443
9 82 79
12 330 331
15 44 -50
18 138-137
21 47 50
24 235 238
27 0 12
30 92 -94
33 35 32*
36 68 64
39 0 -12*
42 75 -71
45 0 12*

H,K= 4, 2
L FOB FCA
2 296-297
5 0 6
8 117 123
11 0 11
14 235-239
17 24 31
20 183 184
23 0 3
26 141-148
29 0 -11*
32 137 136
35 0 7*
38 47 -51
41 0 8*
44 78 89

H,K= 4, 3
L FOB FCA
1 0 -2
4 168 172
7 13 17
10 13 -14
13 14 19
16 204 208
19 39 35
22 169-167
25 0 -2
28 173 173
31 0 10*
34 136-137
37 19 15*
40 112 114
43 0 -6*

H,K= 4, 4
L FOB FCA
0 166 165
3 53 55
6 41 -43
9 14 19
12 168 168
15 21 -33
18 208-206
21 72 68
24 135 133
27 42 -40
30 99-103
33 19 14*
36 140 133
39 20 14*

H,K= 4, 5
L FOB FCA
2 208-214
5 0 -5
8 178 175
11 26 28
14 96 -99
17 0 -3
20 37 36
23 0 4*
26 94 -94
29 0 8*
32 117 114
35 20 -8*
38 55 -61

H,K= 4, 6
L FOB FCA
1 0 1
4 209 210
7 0 13
10 174-174
13 0 -4*
16 111 107
19 25 23*
22 84 -82
25 0 5*
28 125 123
31 0 6*
34 54 -54
37 21 22*

H,K= 4, 7
L FOB FCA
0 133 133
3 0 -3*
6 198-203
9 0 4*
12 131 126
15 0 0*
18 73 -68
21 32 28*
24 105 99
27 0 -10*
30 86 -83
33 0 14*

H,K= 4, 8
L FOB FCA
2 96 -98
5 25 28*
8 72 63
11 0 1*
14 136-137
17 0 -3*
20 126 126
23 20 10*
26 65 -59
29 0 -9*

H,K= 4, 9
L FOB FCA
1 0 -9*
4 97 91
7 0 2*
10 89 -89
13 20 8*
16 132 131
19 0 5*
22 80 -74
25 0 9*

H,K= 4,10
L FOB FCA
0 72 73
3 0 1*
6 76 -84
9 0 4*
12 71 72
15 0 -5*

H,K= 5,-5
L FOB FCA
1 39 -40
4 207 213
7 91 92
10 21 -24
13 0 2
16 157 158
19 14 16
22 221-221
25 0 7
28 214 209
31 0 7
34 175-173
37 27 24*
40 107 115
43 0 -13*

H,K= 5,-4
L FOB FCA
3 0 -1
6 129-132
9 118 119
12 159 163
15 57 -58
18 210-210
21 58 57
24 96 96
27 27 -31
30 129-127
33 17 -1*
36 171 174
39 19 12*
42 72 -70
45 21 15*

H,K= 5,-3
L FOB FCA
2 254-249
5 11 -13
8 401 401
11 86 85
14 152-159
17 0 13

```
 20  45  49
 23  14 -20
 26  88 -86
 29   0  20
 32 142 144
 35   0   8*
 38 115-107
 41  20   8*
 44  87  85

 H,K= 5,-2
 L FOB FCA
  1  44  46
  4 621 616
  7   0  -6
 10 152-152
 13  21  19
 16 196 201
 19  59  61
 22 255-265
 25   0  -6
 28  50  42
 31   0 -12*
 34  80 -84
 37  18  16*
 40 130 139
 43   0  -7*
 46  85 -84

 H,K= 5,-1
 L FOB FCA
  3  72  68
  6 405-394
  9  12  18
 12  89  92
 15  38 -43
 18 278-278
 21  49  52
 24 236 232
 27  47 -53
 30  17 -11
 33  46  46
 36 125 123
 39   0   8*
 42  94 -93
 45   0   2*

 H,K= 5, 0
 L FOB FCA
  2  66 -69
  5  59  49
  8 282 278
 11  43  41
 14 250-251
 17   0   1
 20 282 280
 23  37  32
 26 140-135
 29  16   7*
 32  67  60
 35  18   3*
 38 108-108
 41  20   4*
 44  72  63

 H,K= 5, 1
 L FOB FCA
  1  34 -35
  4 185 186
  7  51  52
 10 188-188
 13   0  -3
 16 269 268
 19  14  18
 22 205-208
 25   0   3
 28 178 176
 31   0   3*
 34 163-161
 37  27  23*
 40  75  73
 43  21 -20*

 H,K= 5, 2
 L FOB FCA
  0 357 357
  3   0  10
  6 143-147
  9  33  35
 12 132 133
 15   0   3
 18 216-216
 21  34  32
 24 111 109
 27  34 -38*
 30  99-100
 33  18  23*
 36 136 133
 39   0  -3*
 42  51 -52

 H,K= 5, 3
 L FOB FCA
  2 108-112
  5  44  47
  8  72  78
 11  25  22
 14  47 -49
 17   0  -3
 20 138 143
 23  37  37
 26 141-139
 29  18  -8*
 32 116 118
 35   0   3*
 38 113-118
 41   0   7*

 H,K= 5, 4
 L FOB FCA
  1   0  -2
  4 190 193
  7   0   2
 10  69 -69
 13  27  30
 16 172 170
 19  23  17*
 22 178-175
 25  18 -17*
 28  97  97
 31   0  -4*
 34  76 -73
 37   0  11*

 H,K= 5, 5
 L FOB FCA
  0 161 163
  3  22  25
  6 143-141
  9  32  28
 12 201 201
 15   0 -20*
 18  87 -93
 21  31  35*
 24 101  92
 27   0 -14*
 30 101-100
 33   0  17*
 36  63  63

 H,K= 5, 6
 L FOB FCA
  2  83 -83
  5  29  29*
  8 184 184
 11   0  -0*
 14  86 -85
 17  18  17*
 20  37  30
 23  19   5*
 26 101 -93
 29   0 -10*
 32  72  64

 H,K= 5, 7
 L FOB FCA
  1  31 -34*
  4  87  85
  7  18  18*
 10 114-112
 13  18  -1*
 16 109 110
 19   0  -7*
 22 100 -95
 25  20  14*
 28 111 108

 H,K= 5, 8
 L FOB FCA
  0 155 158
  3   0   4*
  6 102-101
  9  19   5*
 12  97  94
 15  20  11*
 18 100-100
 21  20  17*
 24  78  81

 H,K= 5, 9
 L FOB FCA
  2  79 -81
  5  20  14*
  8 114 111
 11  20  -0*
 14  62 -58
 17   0  10*

 H,K= 5,10
 L FOB FCA
  1  21  -2*
  4  87  92
  7  21  15*

 H,K= 6,-6
 L FOB FCA
  3  31  29
  6 208-210
  9  23   9
 12 120 128
 15  14   8
 18 134-135
 21  37  30
 24 187 188
 27   0 -21*
 30 114-119
 33  63  48
 36  78  77
 39  20 -20*
 42  85 -89

 H,K= 6,-5
 L FOB FCA
  2  36 -40
  5  53  54
  8 129 133
 11  18  22
 14 199-198
 17   0  10
 20 171 168
 23   0   9
 26 114-118
 29   0  -2*
 32 153 155
 35  26  27*
 38  93 -95
 41   0   9*
 44  67  71

 H,K= 6,-4
 L FOB FCA
  1   0   6
  4  75  77
  7  30  32
 10  30 -37
 13  26 -23
 16 362 359
 19  49  55
 22 111-113
 25   0  11
 28 176 176
 31  17  15*
 34 182-179
 37  27  20*
 40 101  99
 43  21 -25*

 H,K= 6,-3
 L FOB FCA
  3  43  43
  6 167-171
  9  66  67
 12 324 321
 15  37 -36
 18 227-227
 21  80  78
 24  51  46
 27  36 -35
 30 120-118
 33   0   9*
 36 135 131
 39   0   1*
 42  50 -52

 H,K= 6,-2
 L FOB FCA
  2 206-203
  5  37  40
  8 243 242
 11  40  35
 14  23 -27
 17   0 -15
 20 124 130
 23  40  38
 26 102-109
 29   0  11*
 32 145 141
 35   0   6*
 38 110-107
 41   0   8*
 44  84  95

 H,K= 6,-1
 L FOB FCA
  1   0   2
  4 271 271
  7  21  26
 10 198-194
 13  26  28
 16 175 176
 19  14 -10
 22 132-133
 25   0   1
 28 208 205
 31  25  24*
 34 111-109
 37  27  20*
 40  96  93
 43   0  -7*

 H,K= 6, 0
 L FOB FCA
  3  18  -9*
  6  64 -65
  9  25  19*
 12  95  97
 15  19  10*
 18  63 -64
 21  19   8*
 24 114 110
 27  20  -5*
 30  76 -79

 H,K= 6, 1
 L FOB FCA
  2  81 -84
  5  27  27*
  8  65  70
 11  19 -10*
 14  67 -68
 17   0   8*
 20 116 111
 23  21  10*
 26  47 -53

 H,K= 6, 2
 L FOB FCA
  1  48 -45
  4 197 205
  7  53  50
 10  52 -57
 13  26  22
 16 214 212
 19   0   7
 22 141-145
 25  24  22*
 28 108 109
 31   0  -8*
 34 120-125
 37   0   6*
 40  84  84

 H,K= 6, 3
 L FOB FCA
  0 227 227
  3  15  26
  6 109-116
  9  26  33
 12 184 185
 15   0  -7
 18 203-200
 21  29  27*
 24 119 117
 27  26 -23*
 30  75 -78
 33  28  26*
 36  95  93
 39  21  -2*

 H,K= 6, 4
 L FOB FCA
  2  98-102
  5  16  15
  8 154 154
 11  16   8*
 14 102-106
 17   0  12*
 20 124 133
 23  18  11*
 26  91 -90
 29   0   9*
 32 115 108
 35  21   7*

 H,K= 6, 5
 L FOB FCA
  1   0 -12*
  4  83  82
  7  38  38
 10 182-179
 13  17  -5*
 16 139 136
 19   0   7*
 22  75 -76
 25   0   6*
 28 117 119
 31   0  -2*
 34  82 -84

 H,K= 6, 6
 L FOB FCA
  0 133 132
  3  18  -9*
  6  64 -65
  9  25  19*
 12  95  97
 15  19  10*
 18  63 -64
 21  19   8*
 24 114 110
 27  20  -5*
 30  76 -79

 H,K= 6, 7
 L FOB FCA
  2  81 -84
  5  27  27*
  8  65  70
 11  19 -10*
 14  67 -68
 17   0   8*
 20 116 111
 23  21  10*
 26  47 -53

 H,K= 6, 8
 L FOB FCA
  1   0 -11*
  4 103 105
  7  20  16*
 10  63 -62
 13   0   6*
 16  62  62
 19   0   1*

 H,K= 6, 9
 L FOB FCA
  0  91  92
  3   0   0*
  6 100-104
  9   0   9*

 H,K= 7,-7
 L FOB FCA
  2 146-147
  5  88  81
  8 231 231
 11   0  -2
 14 110-110
 17  15  -9
 20 136 133
 23  33  37*
 26  81 -80
 29   0 -16*
 32  99  95
 35   0  12*
 38  90 -86
 41  30  12*

 H,K= 7,-6
 L FOB FCA
  1  56 -59
  4 217 222
  7  23  23
 10 239-233
 13  40  38
 16  69  66
 19  34 -36
 22 125-126
 25   0  13*
 28 185 185
 31   0  15*
 34 116-112
 37   0   9*
 40  79  82

 H,K= 7,-5
 L FOB FCA
  3   0   3
  6 201-207
  9  27  30
 12 223 221
 15   0   7
 18 179-184
 21  41  39
 24 132 133
 27  17 -23*
 30  90 -93
 33  37  34*
 36  96  97
 39   0 -12*
 42  47 -50

 H,K= 7,-4
 L FOB FCA
  2 258-254
  5  29  30
  8  97 102
 11  23 -25
 14 227-222
 17   0   5
 20 230 232
 23  16  15
 26  89 -88
 29   0  15*
 32 111 112
 35   0  11*
 38  73 -81
 41   0  -2*

 H,K= 7,-3
 L FOB FCA
  1   0  -1
  4 147 147
  7  58  56
 10 303-296
 13  14 -26
 16 170 166
 19  21  20
 22 148-148
 25  16   7
 28 171 171
 31   0  -2*
 34 101 -97
 37   0  21*
 40 105 103
 43   0 -16*

 H,K= 7,-2
 L FOB FCA
  3  36  38
  6 185-183
  9  13  17
 12 250 247
 15  28 -36
 18  63 -69
 21  51  50
 24 219 220
 27   0   7*
 30 155-157
 33  32  32*
 36  58  56
 39  20 -14*
 42  75 -79

 H,K= 7,-1
 L FOB FCA
  2  29  18
  5  80  78
  8  69  67
 11   0 -10
 14 236-230
 17  15  -2
 20  58  54
 23   0   6
 26 124-122
 29  25 -23*
 32 174 169
 35  27  24*
 38  75 -78
 41   0   6*

 H,K= 7, 0
 L FOB FCA
  1  68 -67
  4 132 131
  7  66  63
 10 252-253
 13   0   1
 16 161 157
 19  38 -28
 22  80 -73
 25  41  40
 28 177 176
 31   0   6*
 34 116-118
 37   0  11*
 40  62  71

 H,K= 7, 1
 L FOB FCA
  0 322 322
  3   0   1
  6 191-186
  9  21   6
 12 176 173
 15  22  20
 18  91 -87
 21  17  20*
 24  73  72
 27  18 -23*
 30  83 -85
 33  39  37*
 36  80  85
 39   0 -11*

 H,K= 7, 2
 L FOB FCA
  2 222-225
  5  26  35
  8 134 138
 11   0 -12
 14 118-121
 17  16   5*
 20 109 103
 23  18   6*
 26 101 -99
 29   0   1*
 32  85  81
 35   0   3*
 38  47 -44

 H,K= 7, 3
 L FOB FCA
  1  16   6
  4 143 144
  7  56  52
 10 152-150
 13  29 -27*
 16 171 171
 19  25  27*
 22 130-128
 25   0   5*
 28 107 110
 31   0  -7*
 34  68 -72

 H,K= 7, 4
 L FOB FCA
  0 106 102
  3   0 -20*
  6 121-122
  9  38  38
 12 214 217
 15  18 -20*
 18 130-133
 21  19  10*
 24  83  80
 27   0   5*
 30  84 -87
 33   0   7*

 H,K= 7, 5
 L FOB FCA
  2  40 -34
  5  25  26*
  8  57  52
 11  18 -11*
 14 145-145
 17  19   3*
 20  55  56
 23   0  -6*
 26  67 -64
 29   0  -1*

 H,K= 7, 6
 L FOB FCA
  1   0 -16*
  4  92  89
  7  19  11*
 10  81 -76
 13   0   4*
 16  71  72
 19   0   4*
 22  82 -84
 25   0  10*

 H,K= 7, 7
 L FOB FCA
  0 106 113
  3  20   7*
  6 101-100
  9   0   9*
 12  57  52
 15   0 -10*
 18  78 -75
 21   0  11*

 H,K= 7, 8
 L FOB FCA
  2  69 -71
  5  21   7*
  8  86  87
 11   0   2*

 H,K= 8,-8
 L FOB FCA
  1   0  -3
  4 275 271
  7  48  40
 10 124-120
 13   0  13
 16 107 102
 19   0  -9*
 22 115-115
 25  25  14*
 28  98  97
 31  33   3*
 34  99 -98
 37   0   5*

 H,K= 8,-7
 L FOB FCA
  3  35  32
  6 250-252
  9  15 -26
 12 179 182
 15   0  13
 18 117-120
 21  62  58
 24  84  79
 27  36 -44*
 30  64 -67
 33  39  35*
 36  67  67
 39   0 -11*

 H,K= 8,-6
 L FOB FCA
  2 226-234
  5  56  61
  8 103 105
 11   0  -2
 14 163-168
 17   0   1
 20 179 179
 23  29  28*
 26  42 -45
 29   0  -5*
 32  88  89
 35   0   7*
 38  70 -73
 41   0   6*

 H,K= 8,-5
 L FOB FCA
  1  53 -48
  4 222 223
  7  71  71
 10  99-100
 13  15 -14
 16 327 331
 19  31  37
 22 208-211
 25  29  34*
 28  66  63
 31  26 -26*
 34 133-130
 37   0  11*
 40  66  72

 H,K= 8,-4
 L FOB FCA
  3  24 -29
  6 262-261
  9  45  46
 12 212 204
 15  33 -17
 18 181-186
 21   0  -3
 24 191 189
 27  25  17*
 30 101 -99
 33   0  23*
 36  78  76
 39  20 -23*

 H,K= 8,-3
 L FOB FCA
  2  34 -45
  5  37  41
  8 148 144
 11  14 -20
 14  59 -63
 17  38  41
 20 105 111
 23   0  13*
 26 186-187
 29   0  -4*
 32 122 124
 35   0   8*
 38  73 -70
 41   0  -9*

 H,K= 8,-2
 L FOB FCA
  1   0   9
  4 151 151
  7  53  53
 10 161-164
 13  21 -26
 16  65  66
 19   0  12
 22 120-121
 25   0   9*
 28 204 205
 31   0   7*
 34 117-117
 37  20  20*
 40  84  82

 H,K= 8,-1
 L FOB FCA
  3   0   6
  6 149-149
  9  21  26
 12 160 162
 15   0  -9
 18 113-113
 21  29  32*
 24 157 154
 27   0 -17*
 30  85 -79
 33  19  23*
 36  85  84
 39   0  -5*

 H,K= 8, 0
 L FOB FCA
  2 126-127
  5  58  58
  8 215 209
 11   0  -9
 14 119-120
 17  16  13*
 20  75  81
 23  25  19*
 26  79 -72
 29   0  -3*
 32  58  58
 35   0   7*
 38  96 -93

 H,K= 8, 1
 L FOB FCA
  1  22 -25
  4 207 213
  7  42  36
 10 155-159
 13   0 -10*
 16 102 102
 19  24   8*
 22 113-123
 25  18  12*
 28 114 118
 31   0  -4*
 34  73 -75
 37   0  12*

 H,K= 8, 2
 L FOB FCA
  0  94  91
  3  16  -9
  6 249-245
  9  33  33*
 12 137 143
 15  30 -27*
 18  59 -49
 21  18  22*
 24 151 149
 27  19  12*
 30  87 -81
 33   0  10*

 H,K= 8, 3
 L FOB FCA
  2  56 -59
  5  17  10*
  8 129 129
 11   0   8*
 14  82 -86
 17  26  29*
 20 119 117
 23   0  -9*
 26 118-118
 29   0   9*
 32  47  51

 H,K= 8, 4
 L FOB FCA
  1   0   9*
  4 100 103
  7  26  26*
 10 114-116
 13  19 -24*
 16 110 116
 19   0   9*
 22  52 -53
 25   0  11*
 28  86  84

 H,K= 8, 5
 L FOB FCA
  0 131 135
  3  19  14*
  6  89 -88
  9  19  15*
 12 106 104
 15   0  -6*
 18  80 -82
 21   0  17*
 24  86  78

 H,K= 8, 6
 L FOB FCA
  2  52 -50
  5   0  14*
  8  96  99
 11   0   5*
 14  61 -66
 17   0  -6*
 20  60  57

 H,K= 8, 7
 L FOB FCA
  1   0   3*
  4  72  77
  7   0   4*
 10  79 -85

 H,K= 9,-9
 L FOB FCA
  3  23  -9
  6 101 -99
  9  16  18*
 12 198 195
 15   0  -4*
 18 109-108
 21  18  22*
 24 110 106
 27   0  -0*
 30  84 -86
 33  20  13*
 36  76  70

 H,K= 9,-8
 L FOB FCA
  2  58 -63
  5  27  30
  8 155 154
 11  16  21
 14 163-165
 17  17   8*
 20  42  43
 23   0   9*
 26  87 -82
 29  19 -11*
 32 103 110
 35   0   1*

 H,K= 9,-7
 L FOB FCA
  1   0  -8
  4 101 102
  7   0   7
 10 112-112
 13   0   5
 16 214 213
 19   0  26*
 22  58 -54
 25   0  11*
 28 139 137
 31   0   6*
 34  98-108
 37   0  11*

 H,K= 9,-6
 L FOB FCA
  3  15 -10
  6 138-133
  9  26  24
 12 122 123
 15   0  -5
 18 153-152
 21  17  22*
 24 126 126
 27   0 -11*
 30 103-100
 33   0  16*
 36  84  84
 39  21  -6*

 H,K= 9,-5
 L FOB FCA
  2 258-256
  5  33  28
  8  70  67
 11  37 -42
 14  65 -64
 17  43  44
 20 195 193
 23  17  24*
 26  89 -84
 29   0   4*
 32  61  60
 35   0  15*
 38  90 -91

 H,K= 9,-4
 L FOB FCA
  1  21 -17
  4 161 158
  7  77  77
 10 172-170
 13  44 -38
 16 214 214
 19  23  19*
 22  56 -57
 25  31  31*
 28 113 108
```

```
31   0 -17*
34  93 -97
37  21  21*

 H,K= 9,-3
 L FOB FCA
 3  21 -23
 6 193-199
 9  55  55
12 224 223
15  16 -26
18 105-106
21  29  32*
24  78  81
27   0   1*
30  94-104
33   0   5*
36  58  58
39   0 -10*

 H,K= 9,-2
 L FOB FCA
 2  99 -97
 5   0   3
 8 153 154
11  16  11
14 142-138
17  16  16*
20 150 145
23   0   3*
26  96 -98
29   0  16*
32  98  98
35   0   2*
38  51 -51

 H,K= 9,-1
 L FOB FCA
 1   0   3
 4 153 155
 7   0   0
10 118-115
13   0  -4*
16 200 199
19  38  36
22 167-165
25   0  -1*
28 117 119
31   0  -4*
34  64 -62
37  21  16*

 H,K= 9, 0
 L FOB FCA
 0 136 136
 3  16  21
 6 176-174
 9  16  14*
12 105 100
15  17 -16*
18 138-130
21  40  37
24 147 141'
27   0 -14*
30  81 -78
33   0  15*
36  73  77

 H,K= 9, 1
 L FOB FCA
 2 122-125
 5   0   8*
 8 115 118
11   0  -2*
14  17  19
17  18  16*
20 135 134
23  19  22*
26 101-105
29   0   4*
32  72  77

 H,K= 9, 2
 L FOB FCA
 1   0   6*
 4  97 101
 7  30  33*
10  96 -94
13  26 -20*
16  82  83
19  19   9*
22 107-109
25   0   7*
28  89  88
31   0  -7*

 H,K= 9, 3
 L FOB FCA
 0 164 165
 3   0 -15*
 6 147-146
 9  26  20*
12  92  90
15  19 -15*
18  93 -93
21   0  18*
24  89  81
27   0   3*

 H,K= 9, 4
 L FOB FCA
 2 118-122
 5  19   5*
 8  72  80
11   0  -0*
14  56 -56
17   0   9*
20  76  81
23   0   7*

 H,K= 9, 5
 L FOB FCA
 1   0   5*
 4 113 113
 7   0   4*
10  97 -95
13   0   2*
16  59  66
19   0   6*

 H,K= 9, 6
 L FOB FCA
 0  62  68
 3   0  11*
 6  72 -79
 9   0   2*

 H,K=10,10
 L FOB FCA
 2  81 -83
 5  17  23*
 8 159 161
11  35 -11*
14  72 -68
17  37  35*
20  75  76
23  19  -3*
26 119-111
29   0  -6*
32  67  70

 H,K=10,-9
 L FOB FCA
 1   0  -9*
 4  62  63
 7  24  27*
10 196-194
13  25 -19*
16 151 149
19  18  14*
22 118-115
25   0   1*
28 114 117
31   0 -10*
34  60 -56

 H,K=10,-8
 L FOB FCA
 3  16  12
 6  73 -68
 9  33  32*
12 220 222
15  17 -13*
18 113-111
21  44  43
24  75  73
27  27 -20*
30 109-107
33   0   1*

 H,K=10,-7
 L FOB FCA
 2  81 -82
 5  16 -13
 8 124 122
11  16   8*
14  75 -75
17   0  11*
20  87  87
23  18   8*
26 106-105
29   0   3*
32 105 103
35   0   0*

 H,K=10,-6
 L FOB FCA
 1   0 -12
 4 113 107
 7  28  25
10 141-145
13   0  -2*
16  95  95
19  17  16*
22 143-140
25  18  -5*
28 118 120
31   0  -9*
34  84 -83
37   0  11*

 H,K=10,-5
 L FOB FCA
 3   0  -1
 6 195-194
 9  32  25
12 180 174
15  17 -13*
18  71 -71
21  18  21*
24 114 113
27   0  -5*
30  75 -76
33  29  21*
36  69  66

 H,K=10,-4
 L FOB FCA
 2 125-124
 5   0  13
 8 150 149
11   0  -2*
14 116-119
17  17  19*
20  68  63
23   0 -11*
26  79 -78
29   0   5*
32  75  76
35   0  12*

 H,K=10,-3
 L FOB FCA
 1   0   6
 4 104  97
 7  32  30
10 154-153
13  24 -26*
16 147 144
19  30  32*
22 110-106
25   0   4*
28 109 108
31   0 -16*
34  68 -68

 H,K=10,-2
 L FOB FCA
 3   0   2
 6  88 -79
 9  29  36*
12 199 196
15  24 -12*
18 165-163
21  36  35*
24 101  99
27  27 -17*
30  72 -72
33   0   9*

 H,K=10,-1
 L FOB FCA
 2 151-155
 5   0  -2*
 8  94  97
11  17   8*
14 108-116
17  18 -13*
20 116 112
23  19  15*
26  87 -79
29   0   2*
32  72  78

 H,K=10, 0
 L FOB FCA
 1   0   7*
 4 100 100
 7   0 -11*
10 117-116
13   0  17*
16 133 130
19   0  18*
22  96 -99
25   0  -3*
28  83  85
31   0   7*

 H,K=10, 1
 L FOB FCA
 0  92  88
 3   0   2*
 6 101-104
 9   0  11*
12 106 100
15  19 -11*
18  76 -74
21  34  24*
24 102 104
27   0  -9*
30  90 -90

 H,K=10, 2
 L FOB FCA
 2 135-129
 5   0  16*
 8  53  49
11  19 -12*
14  64 -62
17   0  14*
20 106 106
23   0   1*
26  55 -66

 H,K=10, 3
 L FOB FCA
 1  19  -8*
 4 128 130
 7  28  25*
10  48 -49
13   0  -1*
16  95  97
19   0   6*
22  87 -84

 H,K=10, 4
 L FOB FCA
 0 102 122
 3   0   8*
 6  61 -67
 9   0   3*
12  77  80
15   0 -10*

 H,K=10, 5
 L FOB FCA
 2  73 -75
 5   0  -2*
 8  56  58

 H,K=11,11
 L FOB FCA
 1   0 -10*
 4 155 157
 7  49  42
10 126-123
13  19  -5*
16  84  83
19  20   0*
22  86 -86
25   0   6*
28  92  88

 H,K=11,10
 L FOB FCA
 3   0  -5*
 6 106-105
 9  36  27*
12 183 176
15   0   3*
18 103-102
21   0   9*
24  96  91
27  21  -7*
30  90 -86

 H,K=11,-9
 L FOB FCA
 2  78 -75
 5  17  12*
 8 148 146
11  18  12*
14 112-115
17  19  -3*
20  78  79
23   0   3*
26  87 -85
29   0   7*

 H,K=11,-8
 L FOB FCA
 1  24  20*
 4 129 126
 7   0  -6*
10  84 -78
13   0   2*
16 116 113
19  37  39*
22 133-136
25   0 -14*
28 108 109
31   0   0*

 H,K=11,-7
 L FOB FCA
 3   0  14*
 6 144-144
 9  34  33*
12  87  80
15  35 -33*
18  70 -69
21  37  37*
24 142 138
27   0 -10*
30  84 -87
33   0   8*

 H,K=11,-6
 L FOB FCA
 2 106-105
 5  17  17*
 8 152 155
11   0  14*
14  17 -26
17  18  10*
20 109 106
23  19   7*
26 101 -94
29   0  -1*
32  65  71

 H,K=11,-5
 L FOB FCA
 1   0 -13*
 4 197 196
 7  29  35*
10 137-132
13  17  11*
16  99  93
19  18  -1*
22  97-101
25  19   8*
28  69  63
31   0  -4*
34  94 -91

 H,K=11,-4
 L FOB FCA
 3   0   1*
 6 134-131
 9  24  19*
12 167 170
15  18   5*
18  85 -86
21  26  17*
24  77  74
27  20 -17*
30  61 -57
33  21  19*

 H,K=11,-3
 L FOB FCA
 2 106 -98
 5  24  23*
 8 156 156
11  18   9*
14  80 -85
17  18  12*
20  77  76
23   0   4*
26  92 -90
29   0  -5*
32  78  81

 H,K=11,-2
 L FOB FCA
 1   0   4*
 4 152 153
 7   0   2*
10  79 -83
13   0   7*
16 148 141
19  27  25*
22 134-132
25   0  -2*
28  84  77
31   0  -0*

 H,K=11,-1
 L FOB FCA
 3  18  18*
 6 100 -97
 9  18  16*
12 140 138
15  26 -16*
18  97 -96
21  39  38*
24  85  83
27  21 -22*
30  56 -56

 H,K=11, 0
 L FOB FCA
 2  61 -53
 5  18  13*
 8  97  94
11  27  15*
14  85 -85
17  19  -0*
20  66  62
23   0   4*
26  59 -57

 H,K=11, 1
 L FOB FCA
 1  27 -20*
 4  81  81
 7  19  13*
10  97-105
13  20   1*
16 103 105
19   0   3*
22  69 -74
25   0  10*

 H,K=11, 2
 L FOB FCA
 0  94 101
 3   0  -5*
 6  88 -94
 9   0   8*
12  97  99
15  20  14*
18  72 -72
21   0   3*

 H,K=11, 3
 L FOB FCA
 2  58 -64
 5   0  19*
 8  77  78
11   0  -3*
14  73 -75

 H,K=12,12
 L FOB FCA
 3   0  -3*
 6 102-104
 9  28   9*
12  87  85
15   0  -1*
18  58 -48
21   0   9*

 H,K=12,11
 L FOB FCA
 2  68 -64
 5  27  27*
 8  92  95
11  19   0*
14  71 -69
17   0  -3*
20  61  58
23   0   5*

 H,K=12,10
 L FOB FCA
 1   0  -2*
 4 108 105
 7  19  -1*
10  73 -70
13  19   8*
16 118 113
19   0  12*
22  89 -89
25   0   6*

 H,K=12,-9
 L FOB FCA
 3   0  11*
 6  91 -88
 9  32  27*
12 104 103
15  27 -22*
18  95 -97
21  28  27*
24  70  69
27   0 -15*

 H,K=12,-8
 L FOB FCA
 2 136-131
 5   0   1*
 8 123 123
11  18   8*
14  81 -81
17   0   3*
20  51  57
23  20  -5*
26  65 -61
29   0  14*

 H,K=12,-7
 L FOB FCA
 1   0   1*
 4 175 173
 7  18  12*
10 123-121
13   0   0*
16 101 100
19  19   7*
22 104-103
25  20   3*
28 115 114

 H,K=12,-6
 L FOB FCA
 6 166-167
 9   0   2*
12 100  98
15   0   0*
18 138-133
21  19  12*
24 127 123
27  20 -21*
30  51 -46

 H,K=12,-5
 L FOB FCA
 2  81 -84
 5  40  39
 8  88  88
11   0   8*
14  94 -89
17  19  -2*
20 120 118
23  20  17*
26  70 -76
29   0  -7*

 H,K=12,-4
 L FOB FCA
 1  25 -25*
 4  91  99
 7  31  21*
10  37 -37
13   0   9*
16 112 113
19   0  -4*
22  97-101
25  20   6*
28 102 110

 H,K=12,-3
 L FOB FCA
 3   0   2*
 6  95 -92
 9  18  15*
12  70  67
15   0  -8*
18  89 -93
21  20  17*
24  64  65
27   0  -8*

 H,K=12,-2
 L FOB FCA
 2 133-134
 5  19   3*
 8 109 108
11  19   6*
14  51 -51
17   0  10*
20  60  60
23  20  -2*
26  36 -36

 H,K=12,-1
 L FOB FCA
 1   0   1*
 4 111 112
 7   0  10*
10  99 -99
13   0  -5*
16  87  94
19   0  12*
22  55 -52
25   0   2*

 H,K=12, 0
 L FOB FCA
 0  98 102
 3   0   3*
 6 118-112
 9  28  11*
12  96  97
15   0  -1*
18  75 -73
21   0  10*

 H,K=12, 1
 L FOB FCA
 2  45 -41
 5  20  25*
 8 115 120
11   0  -1*
14  81 -82
17   0   4*

 H,K=12, 2
 L FOB FCA
 1   0 -11*
 4  55  63
 7   0  10*
10  85 -85

 H,K=13,13
 L FOB FCA
 5  29  11*
 8  78  78
11   0   5*

 H,K=13,12
 L FOB FCA
 1   0 -15*
 4  49  50
 7   0   6*
10  71 -76
13   0   4*
16  47  53

 H,K=13,11
 L FOB FCA
 3  20  13*
 6  91 -88
 9   0   3*
12  67  65
15   0  -1*
18  62 -67
21   0  17*

 H,K=13,10
 L FOB FCA
 2 104-113
 5  19  17*
 8  68  73
11   0   1*
14  49 -49
17   0   5*
20  75  76
23   0   6*

 H,K=13,-9
 L FOB FCA
 1   0  -1*
 4 111 112
 7  19  15*
10  99 -97
13  20 -17*
16  96  94
19   0   7*
22  75 -77
25   0  12*

 H,K=13,-8
 L FOB FCA
 3   0   4*
 6  98 -96
 9   0  15*
12 102  98
15   0  -4*
18 106-100
21  20  14*
24  83  80

 H,K=13,-7
 L FOB FCA
 2  53 -54
 5  27  28*
 8 103 105
11   0   2*
14 101-108
17   0  -5*
20 103 100
23   0   7*
26  63 -67

 H,K=13,-6
 L FOB FCA
 1   0  -5*
 4  94  93
 7  19  11*
10  93 -93
13   0   9*
16  90  85
19  20  -8*
22 117-111
25   0  -4*

 H,K=13,-5
 L FOB FCA
 3   0   9*
 6  65 -65
 9   0   9*
12  88  86
15   0   1*
18  82 -81
21   0  14*
24  78  78

 H,K=13,-4
 L FOB FCA
 2  80 -87
 5  19  25*
 8  64  65
11   0 -11*
14  68 -68
17   0   7*
20  61  59
23   0   2*

 H,K=13,-3
 L FOB FCA
 1   0  -5*
 4 100 102
 7  34  26*
10  81 -76
13   0  -8*
16  99  95
19   0   1*
22  70 -74

 H,K=13,-2
 L FOB FCA
 3   0   3*
 6  79 -81
 9  20  20*
12  73  79
15   0 -14*
18  91 -89
21   0   8*

 H,K=13,-1
 L FOB FCA
 2  75 -74
 5   0  -2*
 8  61  58
11   0  -1*
14  75 -78
17   0   1*

 H,K=13, 0
 L FOB FCA
 1   0  -4*
 4  69  71
 7  21  15*
10  79 -86

 H,K=14,12
 L FOB FCA
 2  51 -50
 5   0  19*
 8  56  51

 H,K=14,11
 L FOB FCA
 1   0  -6*
 4  82  83
 7   0  10*
10  51 -55
13   0   4*

 H,K=14,10
 L FOB FCA
 3   0   6*
 6  86 -87
 9   0   7*
12  80  79
15   0  -7*

 H,K=14,-9
 L FOB FCA
 2  82 -79
 5  20  13*
 8  53  55
11   0  -8*
14  77 -72
17   0   8*

 H,K=14,-8
 L FOB FCA
 1  20  -3*
 4  68  82
 7  20  22*
10  92 -86
13   0 -10*
16  87  90
19  21   6*

 H,K=14,-7
 L FOB FCA
 3   0  -5*
 6  99 -97
 9  20   9*
12  88  87
15   0  -3*
18  75 -71
21  21  14*

 H,K=14,-6
 L FOB FCA
 2  76 -72
 5   0  16*
 8  87  84
11   0   4*
14  84 -79
17   0   7*
20  87  81

 H,K=14,-5
 L FOB FCA
 1   0  -7*
 4  69  60
 7   0  14*
10  78 -79
13   0  -0*
16  90  92
19   0  -3*

 H,K=14,-4
 L FOB FCA
 3   0   2*
 6  78 -78
 9   0   8*
12 105 109
15   0  -2*

 H,K=14,-3
 L FOB FCA
 2  71 -75
 5   0  14*
 8  55  58
11   0  -6*
14  63 -61

 H,K=14,-2
 L FOB FCA
 1  21   2*
 4  86  89
 7   0  19*
10  56 -53

 H,K=15,10
 L FOB FCA
 1   0  -4*
 4  51  60
 7   0  21*

 H,K=15,-9
 L FOB FCA
 3   0  -4*
 6  51 -46
 9   0  10*

 H,K=15,-8
 L FOB FCA
 2  46 -47
 5   0   6*
 8  47  54
11   0 -10*

 H,K=15,-7
 L FOB FCA
 1   0  -2*
 4  75  76
 7   0   9*
10  70 -76

 H,K=15,-6
 L FOB FCA
 3   0   1*
 6 100 -99
 9   0  -0*

 H,K=15,-5
 L FOB FCA
 2  51 -60
 5   0   8*
 8  60  60
```

Table III. Atomic coordinates from least-squares refinement. Standard deviations are $\sigma(x) = \sigma(y) = 0.0005$ for O and N, $\sigma(z) = 0.0001$ for Mg(2), O, and N, and $\sigma(z) = 0.00002$ for Ce.

Atom[a]	x	y	z
Ce	0	0	0.24966
Mg(1)	0	0	0
Mg(2)	0	0	0.4279
O(N11)	-0.0563	0.1202	0.3089
O(N12)	0.0441	0.3454	0.3185
O(N13)	0.1088	0.2614	0.2712
O(N21)	0.1256	0.1782	0.1926
O(N22)	0.3500	0.3044	0.1844
O(N23)	0.2650	0.1526	0.2310
O(W1)	0.0128	0.1576	0.0349
O(W2)	0.1607	0.0173	0.3938
O(W3)	0.1567	0.1548	0.4609
O(W4)	0.1669	0.2282	0.1044
N(1)	0.0316	0.2450	0.3002
N(2)	0.2495	0.2136	0.2023
H(1W2)	0.0554	0.1962	0.0524
H(2W1)	-0.0065	0.2062	0.0278
H(1W2)	0.1761	0.0500	0.3813
H(2W2)	0.1649	-0.0535	0.3976
H(1W3)	0.2337	0.1977	0.4550
H(2W3)	0.1418	0.1874	0.4734
H(1W4)	0.2131	0.1871	0.1114
H(2W4)	0.1171	0.2006	0.1237

[a]Atom O(N*ij*) is bonded to N(*i*); H(*i*W*j*) is bonded to O(W*j*).

Table IV. Anisotropic thermal parameters (each $\times 10^5$).

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ce	433	(433)[a]	28	(217)	(0)	(0)
Mg(1)	600	(600)	41	(300)	(0)	(0)
Mg(2)	582	(582)	31	(291)	(0)	(0)
O(N11)	582	620	48	136	33	7
O(N12)	1012	672	67	457	20	-85
O(N13)	631	496	51	226	54	5
O(N21)	502	1027	50	337	13	65
O(N22)	725	1104	71	157	37	130
O(N23)	623	889	42	408	27	73
O(W1)	1112	742	54	526	-43	-54
O(W2)	874	712	51	493	42	14
O(W3)	844	824	63	325	-26	-100
O(W4)	1103	1137	61	733	-11	-3
N(1)	474	618	32	290	25	-7
N(2)	426	568	46	168	23	3

[a] Parentheses indicate parameters which are subject to constraints.

Table V. Isotropic thermal parameters of hydrogen atoms.

Atom	B, Å^2	Atom	B, Å^2
H(1W1)	3.6	H(1W3)	5.4
H(2W1)	4.0	H(2W3)	0.7
H(1W2)	1.3	H(1W4)	1.8
H(2W2)	1.2	H(2W4)	3.2

Table VI. Ce—O distances.

Atoms	Distance,[a] Å (uncorrected)	Distance,[b] Å (corrected)
Ce—O(N11)	2.675	2.680
Ce—O(N13)	2.612	2.616
Ce—O(N21)	2.636	2.643
Ce—O(N23)	2.616	2.622
Ave.	2.635	2.642

[a]Standard deviations are 0.005 Å.

[b]Corrected for thermal motion with assumption that O rides on Ce.

Table VII. Bond distances in nitrate ions.

Atoms	Distance,[a] Å (uncorrected)	Distance,[b] Å (corrected)
N(1)—O(N11)	1.259	1.270
N(1)—O(N12)	1.220	1.242
N(1)—O(N13)	1.268	1.272
N(2)—O(N21)	1.262	1.273
N(2)—O(N22)	1.225	1.251
N(2)—O(N23)	1.257	1.268
Ave.	1.248	1.263

[a]Standard deviations are 0.008 Å.

[b]Corrected for thermal motion with assumption that O rides on N.

Table VIII. Mg—O distances.

Atoms	Distance,[a] Å (uncorrected)	Distance,[b] Å (corrected)
Mg(1)—O(W1)	2.058	2.067
Mg(2)—O(W2)	2.056	2.061
Mg(2)—O(W3)	2.058	2.070
Ave.	2.057	2.066

[a]Standard deviations are 0.005 Å.

[b]Corrected for thermal motion with assumption that O rides on Mg.

Table IX. Hydrogen-bond distances.

Atoms	O—O distance,[a] Å
O(W1)—H(1W1)—O(W4)	2.82
O(W1)—H(2W1)—O(N12)	2.98
O(W2)—H(1W2)—O(N11)	2.96
O(W2)—H(2W2)—O(N13)	2.78
O(W3)—H(1W3)—O(W4)	2.81
O(W4)—H(1W4)—O(N23)	2.88
Ave.	2.87

[a]Standard deviations are less than 0.01 Å.

Table X. Some bond angles.

Atoms	Angle
O(W4)—O(W1)—O(N12)	124°
O(N11)—O(W2)—O(N13)	98°
O(W4)—O(W1)—Mg(1)	121°
O(N12)—O(W1)—Mg(1)	108°
O(N11)—O(W2)—Mg(2)	125°
O(N13)—O(W2)—Mg(2)	112°
O(W4)—O(W3)—Mg(2)	120°
O(N23)—O(W4)—O(W1)	114°
O(N23)—O(W4)—O(W3)	94°

(Figure captions)

Fig. 1. Crystal structure of $Ce_2Mg_3(NO_3)_{12}.24H_2O$. Atoms of Ce and Mg which lie in a section parallel with c and [$\bar{1}$10] are shown, together with the nitrate ions and water molecules near this section. Examples are shown of each kind of hydrogen atom and bond.

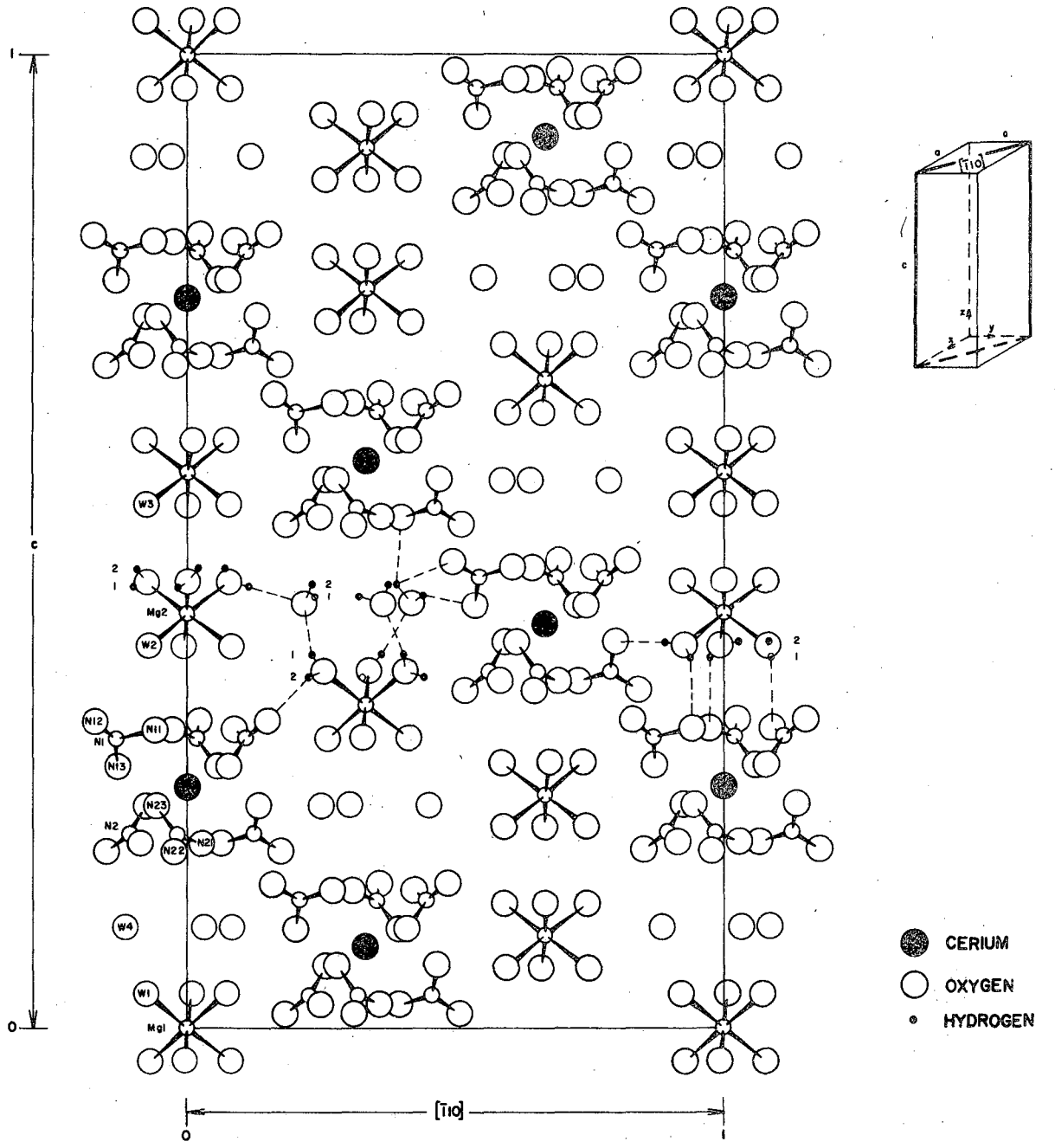
Fig. 2. The magnesium environment of the Ce atom. Distances are in Å.

Fig. 3. The coordination of the Ce atom by nitrate ions, viewed along the 3-fold axis. Alternate nitrate ions are above and below the Ce atom.

Fig. 4. The cerium environment of the Mg(1) atom (at origin). Distances are in Å.

Fig. 5. The cerium environment of a pair of Mg(2) atoms. Distances are in Å.

Fig. 6. Environment of fourth water molecule showing proximity of H(2W4) to two oxygen atoms. Distances (in Å) are those calculated from the coordinates of H atoms found by least squares.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N12
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a
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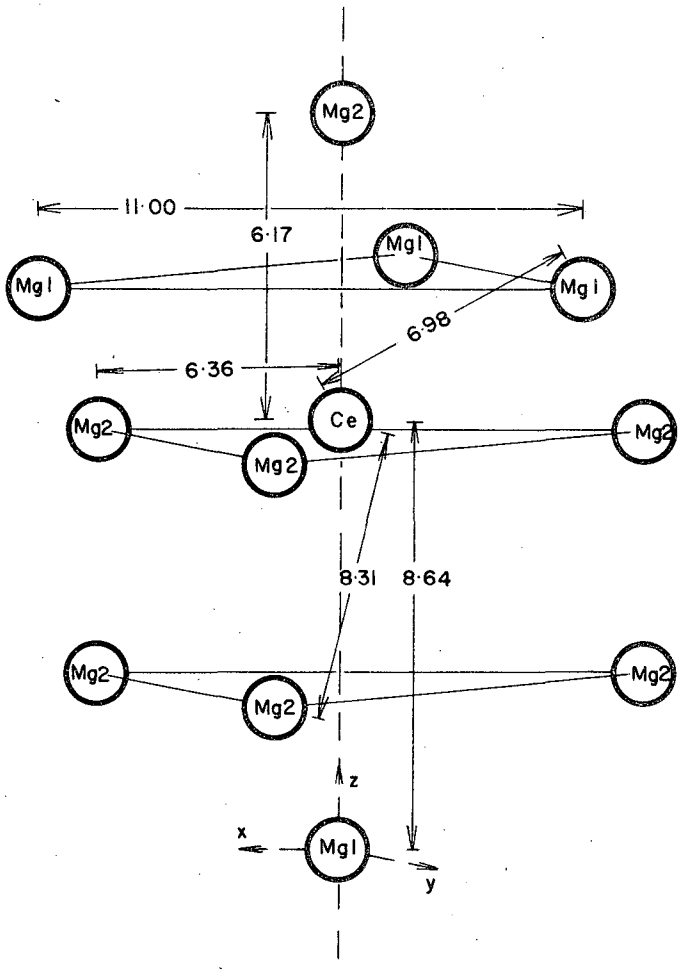
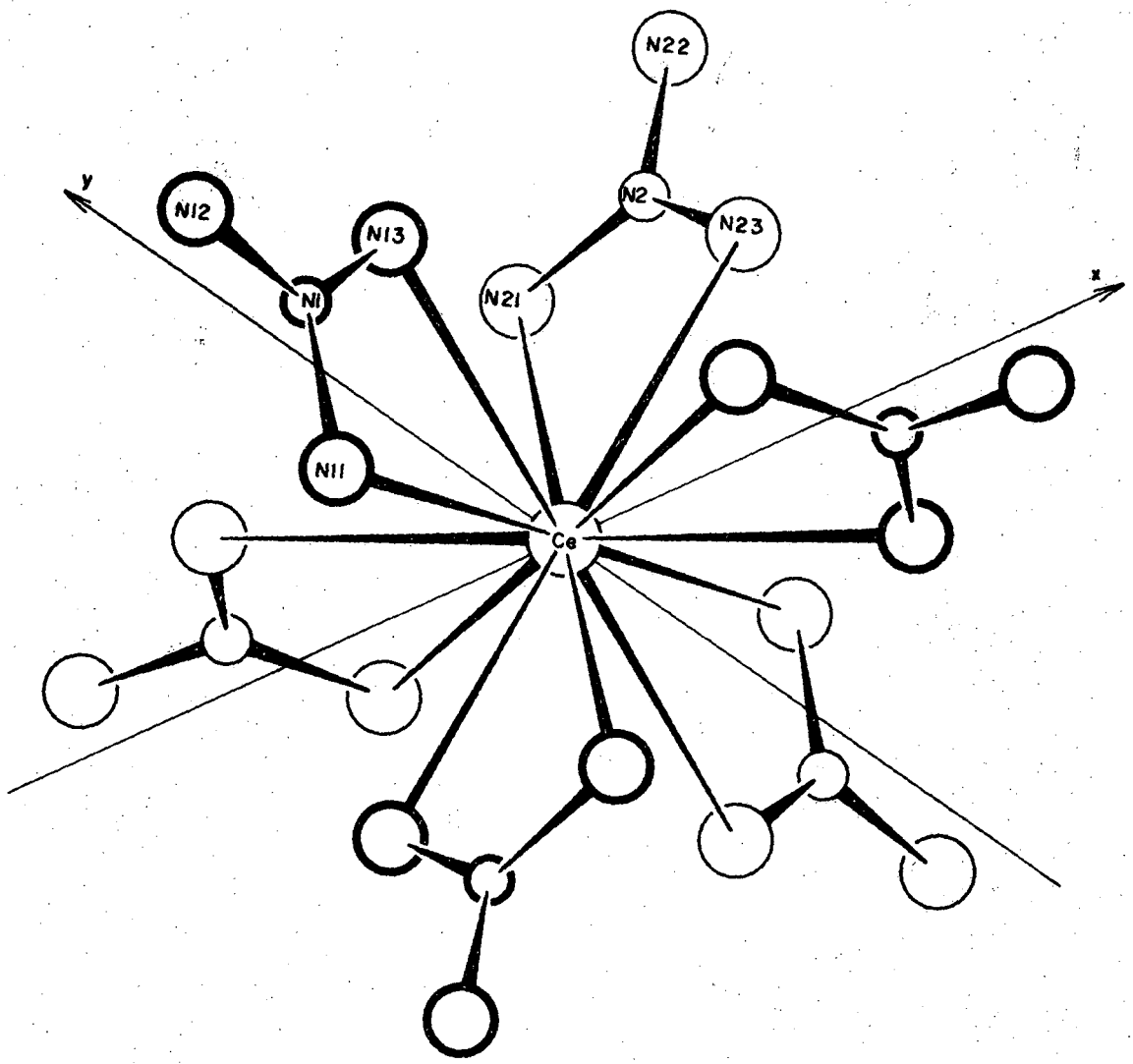
CERIUM
OXYGEN
HYDROGEN
MUB-1437

Fig. 1



MU-28593

Fig. 2



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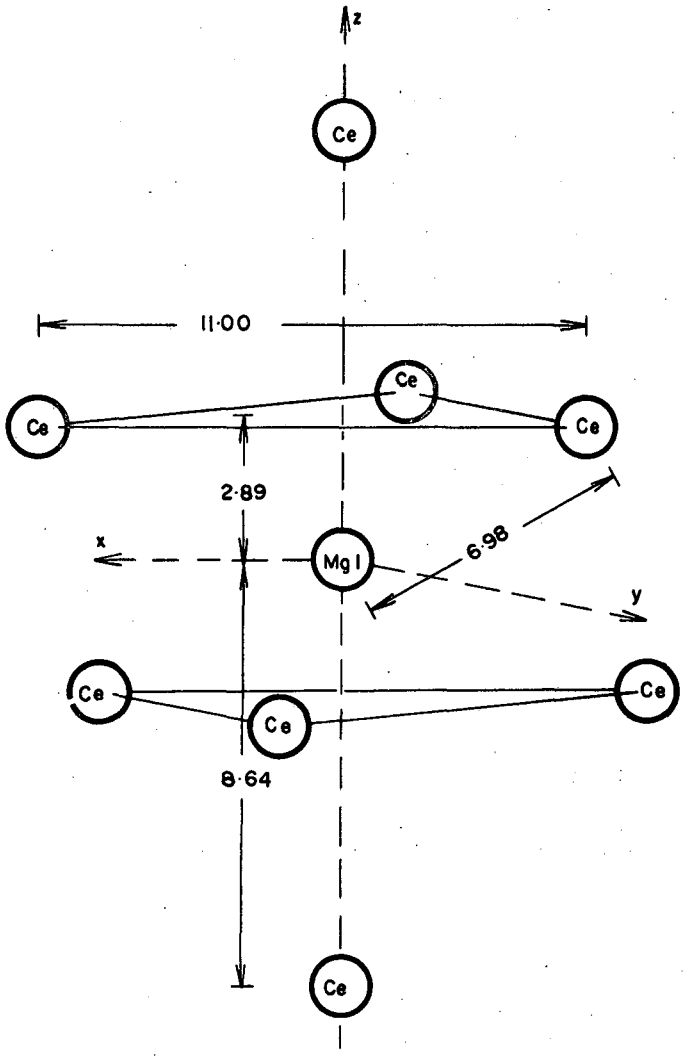

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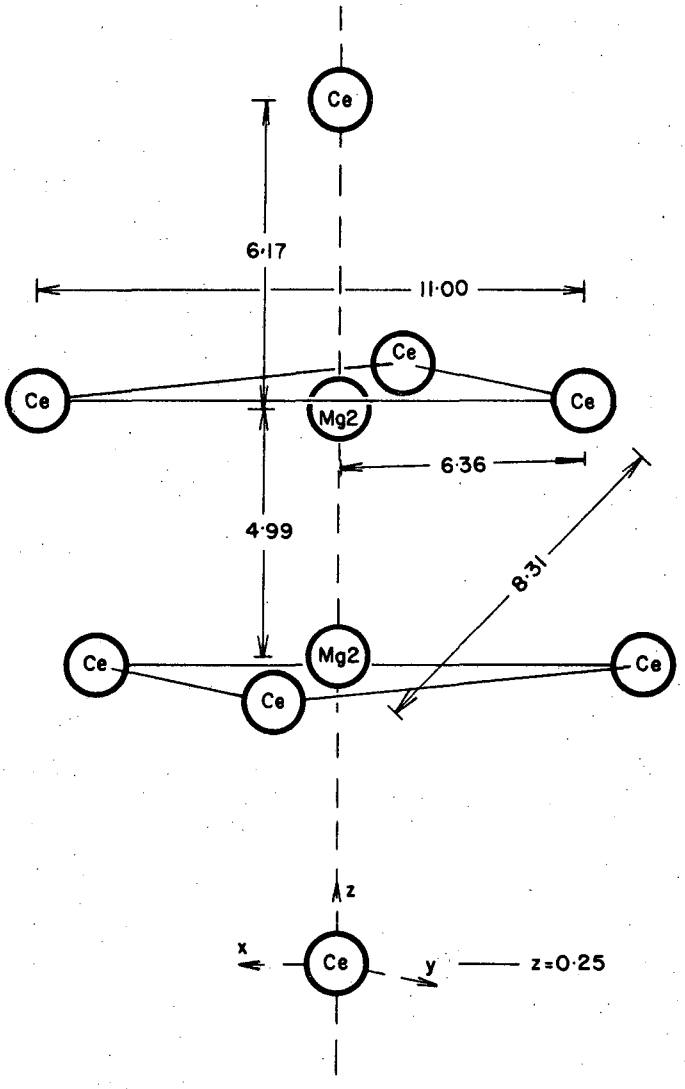
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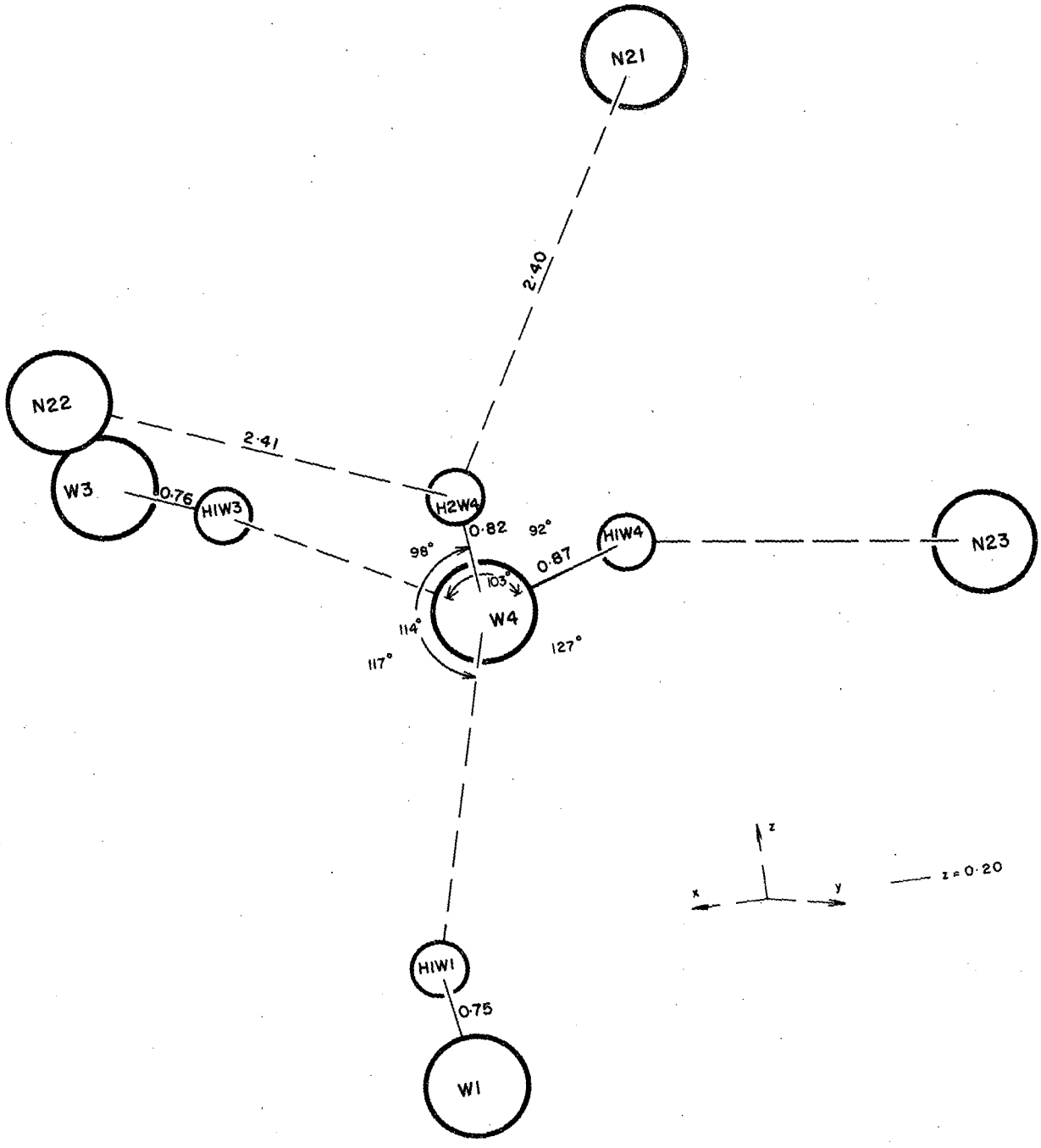
Fig. 5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N23
W4
114°
117°
127°
z
x
y
z = 0·20
HIW1
0·75
W1
MUB-1435

Fig. 6

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