It is apparent that no gain in accuracy resulted from the measurement of a second set of intensities at a reduced temperature. The two possible reasons for this are, firstly, the formation of ice around the crystal, and secondly, the fact that the cooling apparatus was modified during the course of measurement. The reduced temperature determination was partly successful, however, in that it increased the number of available intensities, and reduced the errors arising from the librational corrections.

A complete list of observed and calculated structure amplitudes is given in Table 10.

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The Crystal and Molecular Structure of Newberyite, $MgHPO_4.3H_2O$

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Newberyite, $MgHPO_4.3H_2O$, from Skipton Caves, Victoria, Australia, belongs to the orthorhombic space group *Pbca* with eight molecules in a unit cell of dimensions $a=10\cdot215$, $b=10\cdot681$, $c=10\cdot014$ Å, all $\pm 0\cdot002$ Å. The crystal structure has been determined by Patterson projections and Fourier syntheses, and refined by three-dimensional least-squares methods to an R value of 0·044. The standard deviation in P–O and Mg–O bonds is 0·005 Å. In the phosphate group P–OH is 1·588 Å, the other P–O distances are 1·545, 1·542, 1·500 Å, and most of the O–P–O angles deviate considerably from the tetrahedral value. The distortion probably results from the participation of three phosphate oxygen atoms in the octahedral coordination of magnesium atoms. The Mg–O distances fall into two groups depending on whether the oxygen belongs to a water molecule or a phosphate group. In the latter case, the Mg–O bonds (mean value 2·049 Å) are significantly shorter than in the former (mean 2·118 Å) and probably are of greater ionic character. The crystal structure is very closely packed, with many short O···O contacts, some of which are hydrogen bonds.

Introduction

Newberyite or magnesium hydrogen orthophosphate trihydrate, $MgHPO_4.3H_2O$, is a naturally occurring mineral. It was first identified as a new species in Skipton Caves, Victoria, Australia, where it occurs as large crystals in bat guano. Other well-known deposits also associated with guano are in Mejillones, Chile, Ascension Island and the Tunnel du Comeran in Réunion. An unusual deposit in crystal relics of what was originally struvite has recently been found in Paoha Island, Mono Lake, California (Cohen & Ribbe, 1966). Parsons (1956) identified newberyite as a constituent of a urinary calculus and its occurrence in a few calculi has subsequently been reported elsewhere. We have found it a common constituent of certain collections of calculi studied in this laboratory, *e.g.* 57% of the stones from a collection of (allegedly) modern Indonesian bladder calculi and 31% of the stones examined from the Norwich Hospital Museum Collection of 19th-century bladder calculi contain newberyite (Lonsdale & Sutcr, 1966).

In many of the deposits both mineral and biological, struvite is associated with newberyite, and at Paoha Island the original struvite morphology, preserved by a coating of monetite, indicates that decomposition of struvite to newberyite has occurred. Whether newberyite is ever deposited as such or is always formed by the decomposition of struvite is not yet known. We are investigating the change as part of a research project on the structure, composition and cause of urinary calculi, and determining how newberyite grows on other stone components. The work necessitates a knowledge of the crystal structures and that of newberyite is reported here.

Experimental

Single crystals of newberyite large enough for X-ray work have not been found in calculi and all attempts to grow them were unsuccessful. A piece off a large crystal from Skipton Caves was kindly provided by the Keeper of Minerals, the British Museum. The Skipton material is among the purest found. The original chemical analyses (MacIvor, 1887) showed the amounts of FeO and MnO to be 0·85 and 0·21% respectively and an electron probe analysis (Cohen & Ribbe, 1966) indicated Mg replaced by 0·36 wt.% of Mn but did not detect Fe. The effect on the cell dimensions *etc.* is negligible.

The fragment had perfect (010) cleavage but was difficult to cut in other directions, and only specimens elongated along *c* but of small uniform cross-section could be obtained. Unit-cell dimensions were determined from oscillation photographs using the Ieviņš–Straumanis mounting and Cu *K* radiation: $\lambda = 1{\cdot}54051(\alpha_1)$, $1{\cdot}54433(\alpha_2)$, $1{\cdot}3922\ (\beta_1)$, (Lonsdale & Sutor, 1966).

$$a = 10{\cdot}215,\ b = 10{\cdot}681,\ c = 10{\cdot}014\ \text{Å, all}\ \pm 0{\cdot}002\ \text{Å}\ .$$

Cohen & Ribbe (1966) have obtained accurate cell dimensions for the Skipton material in excellent agreement with ours, and Pollman (1961) measured the cell dimensions of Mejillones newberyite.

Absent spectra are *hk*0 (*h*00) with *h* odd, *h*0*l* (00*l*) with *l* odd and 0*kl* (0*k*0) with *k* odd; space group *Pbca*. The density calculated for eight molecules in the unit cell is 2·119 g.cm^{-3} and the measured density is 2·123 g.cm^{-3} (Groth, 1908). The absorption coefficient for Cu is 29·8 cm^{-1}.

Practically all data within the limiting sphere were recorded on Weissenberg photographs *hk*0–*hk*9 with Cu *K* radiation and equi-inclination angles up to 45°. Data collected about axes other than *c* varied in spot-shape because of the non-uniform cross-section of the cut crystals, and only the *h*0*l* and 0*kl* layers were photographed. The multiple-film technique was employed and frequently three film packs of three films were necessary to reduce reflexions to a measurable intensity. Intensities of the α reflexions were measured visually by comparison with a standard scale and the probable error in each estimation noted. Structure amplitudes were computed with the Intensity Processing Program for Pegasus (D. Milledge, H. J. Milledge & D. Walley, unpublished). The program scales and averages the data taking into account the errors in intensity measurements, applies the usual corrections and prints out $|F_o|$ together with the range derived from the errors in the scaled data, representing the most probable region in which $|F_o|$ lies. No absorption corrections were made. The *hk*0–*hk*9 layers were placed on the same arbitrary scale using the *h*0*l* data corrected approximately for spot-shape and scale factors derived as above. In all, 1118 reflexions were obtained, all of which were of measurable intensity.

Determination of the structure

The *hk*0, *h*0*l* and 0*kl* Patterson projections sharpened by using $|F_o|$ values instead of F_o^2 were calculated on Pegasus with the structure-factor least-squares program (Milledge, 1962) which will compute Fourier series for a maximum of eighty terms. The *hk*0 projection indicated eight possible arrangements for the *x* and *y* coordinates of magnesium and phosphorus, compatible with the *h*0*l* and in part the 0*kl* projection and with *R* values in the range 55–80%. Fourier syntheses were calculated and that for the arrangement with $R = 55\%$ had maxima in stereochemically acceptable positions for the seven oxygen atoms. Refinement of the coordinates by difference syntheses reduced *R* to 23% for fifty *hk*0 reflexions, but overlap prevented any further improvement.

From the *h*0*l* projection two sets of *z* coordinates for magnesium and phosphorus and relative *z* coordinates of the oxygen atoms could be obtained. One set was stereochemically unacceptable and was ignored; the other was tested by calculating some low-order three-dimensional structure factors. Only the *y* coordinates had been unambiguously determined from the projections and therefore shifts of the molecule of $\frac{1}{4}$ along either *a* and/or *c* had to be tried. For the arrangement having the best agreement between observed and calculated structure factors, *R* was improved from 39 to 11% by three cycles of least-squares. In the process the number of terms was restricted to thirty-five, just in excess of the number of parameters. Once more accurate coordinates were obtained structure factors were calculated for twice the number of reflexions. There was no significant increase in *R*.

Refinement of the structure

The coordinates were refined by the structure-factor diagonal-least-squares program for Pegasus (Milledge, 1962). The quantity minimized was $\Sigma\, w(F_o - F_c)^2$ and throughout *w* was taken as unity. Atomic scattering factors were those listed in *International Tables for X-ray Crystallography* (Ibers, 1962) with the non-ionic form for magnesium. Individual isotropic temperature factors were assigned to each atom and refined by the program. Even if allowance is made for the non-application of absorption corrections, the values of *B* are so small that anisotropic vibration corrections would hardly be significant and were not applied.

To reduce refinement time, reflexions were divided into five blocks with $\sin\theta/\lambda = 0$–0·30, 0·30–0·40, 0·40–0·48, 0·48–0·56, 0·56–0·65. Facilities for the selection of the appropriate reflexions from the master tape of $|F_o|$ are incorporated in the program. Two cycles of least-squares were applied to each block in turn and convergence was reached more rapidly without the damping effect of low-order terms on the outer reflexions and *vice versa*. At the end of the process R was 17·5% for the last block, and after adjustment of the scale factors for individual layer lines, necessary because of the approximate corrections for spot-shape applied to the $0kl$ terms, the overall agreement was 10·4%. One full cycle of least-squares reduced R to 9·2%, beyond which no improvement could be obtained. For the last cycle of refinement, the average positional parameter shift was 0·0012 Å and the maximum 0·0041 Å corresponding to $0·8\sigma$. The maximum thermal parameter shift was $0·9\sigma$.

Structure factors were then calculated and the R index evaluated, taking into account the experimentally determined range R' on $|F_o|$. If $|F_c|$ fell within the range $|F_o| \pm R'$, ΔF was considered zero for that reflexion but the value of $|F_o|$ was added to the denominator of the expression for R. The R value was 4·4%.

No attempt was made to locate the hydrogen atoms by difference syntheses, and the large number of O···O distances which could represent hydrogen bonds prevented unequivocal assignment of hydrogen coordinates on this basis.

The final atomic coordinates, their standard deviations and the isotropic temperature factors for each atom are listed in Table 1. Values of $|F_o|$ and F_c calculated from these coordinates are given in Table 2. Distances and angles in the phosphate tetrahedron and magnesium octahedron are found in Table 3. The standard deviations are 0·005 Å for P–O and Mg–O bonds and 0·007 Å for O···O distances. The standard deviation in the angles O–Mg–O and O–P–O is 0·4° (Darlow, 1960).

Discussion

In the phosphate tetrahedron, the bond P–O(6) of 1·588 Å is significantly longer and P–O(3) at 1·500 Å is significantly shorter than the other two bonds of 1·542 and 1·545 Å. As P–OH distances are longer than P–O, the acidic hydrogen is attached to O(6). This arrangement is confirmed by the very short intermolecular O(4)···O(6) distance of 2·609 Å which must represent a hydrogen bond. The mean of the four P–O distances 1·544 ± 0·002 Å agrees well with values found in other accurately determined phosphate structures, *e.g.* the mean value of 1·537 ± 0·001 Å for the phosphate group in struvite (Whitaker, 1965). In this compound there are no hydrogen atoms attached to the phosphate group and no significant differences in P–O bonds. Therefore, the lengthening of P–O(6) in newberyite is compensated by the shortening of P–O(3).

The angles in the phosphate group apart from O(4)–P–O(5) are significantly different from the tetrahedral value. The three involving O(6) are less, and the other two greater than the tetrahedral angle. Distortion probably results from the participation of phosphate groups in the coordination of magnesium atoms.

The magnesium is coordinated octahedrally by the three water molecules and three oxygen atoms from different phosphate groups (Fig. 1). These oxygen atoms are O(3) at $\frac{1}{2}+x,y,\frac{1}{2}-z$, O(4) at $\frac{1}{2}+x,\frac{1}{2}-y,\bar{z}$ and O(5) at x,y,z. The oxygen carrying the hydrogen atom does not participate in magnesium coordination. The six Mg–O distances fall into two distinct groups:

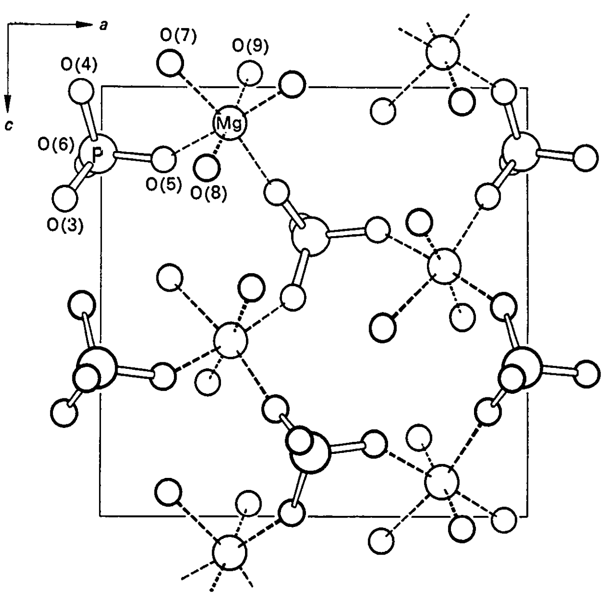

Fig. 1. Bounded projection of the structure from $y = 0 - 0·5$ on (010), showing the magnesium coordination. The magnesium atoms which are approximately coplanar are sandwiched by two planes of phosphorus atoms. In the bounded projection from $y = 0·5 - 1·0$ which completes the structure, the atoms are related to these by $\frac{1}{2}-x$, $\frac{1}{2}+y$, z.

Table 1. *Fractional atomic coordinates with their standard deviations* (*both* × 10^5), *and isotropic temperature factors, with their standard deviations* (× 10^2)

	x	y	z	B
P	−897 (14)	13254 (14)	15364 (16)	0·67 (2) Å^2
Mg	29683 (19)	24666 (19)	8644 (22)	0·72 (3)
O(3)	−8849 (45)	20017 (42)	25682 (52)	1·52 (7)
O(4)	−5097 (44)	16132 (42)	892 (48)	1·30 (7)
O(5)	14006 (42)	15337 (40)	16736 (46)	1·11 (7)
O(6)	−3371 (42)	−1235 (42)	17864 (46)	1·28 (7)
O(7)	16684 (47)	31363 (45)	−6051 (51)	1·69 (8)
O(8)	24894 (49)	41417 (44)	18918 (49)	1·61 (8)
O(9)	35504 (52)	9193 (50)	−3328 (56)	2·16 (9)

Note: P and Mg were designated (1) and (2); hence the numbering scheme for oxygen from (3) to (9).

(1) the three bonds with water molecules of length 2·107, 2·121 and 2·127 Å, (2) the three bonds with phosphate oxygen atoms of length 2·021, 2·053 and 2·073 Å. This division may not be significant, for two reasons. First the effect was not observed in $MgSO_4.4H_2O$ (Baur, 1962, 1964) where magnesium coordination is completed by two sulphate oxygen atoms, but the structure has not been so accurately determined.

Table 2. *Observed and calculated structure factors for* $F(000)=83$ (*one molecule only*)

The values were scaled down to prevent overflow in Pegasus.

H	K	L	F(O)	F(C)
2	0	0	4.96	5.97
4	0	0	7.37	8.12
6	0	0	9.70	9.73
8	0	0	3.33	3.42
10	0	0	3.03	2.41
12	0	0	1.79	1.34
2	1	0	7.39	8.45
4	1	0	7.30	6.38
6	1	0	11.18	12.04
8	1	0	5.90	-5.26
10	1	0	3.00	2.45
12	1	0	3.78	3.62
0	2	0	13.03	-14.95
2	2	0	6.66	7.15
4	2	0	5.99	5.06
6	2	0	1.55	-1.49
8	2	0	6.87	6.12
10	2	0	6.33	-5.92
12	2	0	1.20	1.09
2	3	0	1.42	-1.75
4	3	0	3.60	3.06
6	3	0	6.79	-6.58
8	3	0	8.90	8.41
10	3	0	0.82	0.83
12	3	0	0.50	-0.44
0	4	0	8.61	-9.03
2	4	0	8.30	-9.40
4	4	0	1.25	-1.23
6	4	0	6.57	-6.05
8	4	0	11.34	-11.54
10	4	0	2.84	2.51
12	4	0	6.64	-6.39
2	5	0	7.32	7.12
4	5	0	15.42	-15.04
6	5	0	2.73	-2.41
8	5	0	5.65	-4.95
10	5	0	1.49	-1.55
12	5	0	2.38	-2.00
0	6	0	2.78	2.71
2	6	0	16.40	16.90
4	6	0	2.77	-2.52
6	6	0	3.99	3.62
8	6	0	1.44	0.89
10	6	0	3.57	-3.22
2	7	0	7.67	-7.49
4	7	0	10.31	9.92
6	7	0	4.18	-3.69
8	7	0	1.99	-1.90
10	7	0	2.87	-2.43
0	8	0	9.31	8.43
2	8	0	4.66	4.38
4	8	0	10.33	10.07
6	8	0	7.24	7.08
8	8	0	2.49	2.46
10	8	0	6.69	6.35
2	9	0	0.41	-0.04
4	9	0	5.15	-4.98
6	9	0	7.15	7.22
8	9	0	0.59	-0.45
0	10	0	3.71	-3.78
2	10	0	0.41	0.22
4	10	0	3.39	-3.50
6	10	0	3.56	-3.64
8	10	0	0.39	0.46
2	11	0	0.98	-0.90
4	11	0	2.06	2.18
6	11	0	6.01	-6.02
0	12	0	3.97	3.26
2	12	0	6.95	-7.19
4	12	0	1.45	-1.49
6	12	0	2.48	-2.29
2	13	0	0.93	0.93
4	13	0	3.71	-3.96
1	1	1	7.29	8.15
2	1	1	0.25	0.12
3	1	1	12.83	13.46
4	1	1	9.01	7.98
5	1	1	3.83	3.37
6	1	1	7.11	6.63
7	1	1	0.35	0.08
8	1	1	1.85	1.58
9	1	1	2.18	1.79
10	1	1	2.24	2.38
11	1	1	0.35	0.57
12	1	1	3.27	3.08
0	2	1	12.51	-14.81
1	2	1	0.67	0.73
2	2	1	11.98	-14.06
3	2	1	0.31	-0.09
4	2	1	3.06	2.00
5	2	1	9.38	9.14
6	2	1	9.17	-8.77
7	2	1	4.27	3.99
8	2	1	3.80	-3.53
9	2	1	2.28	0.43
10	2	1	5.11•	-4.87
11	2	1	0.34	0.57
12	2	1	2.75	-2.53
13	2	1	1.93	2.55
1	3	1	6.78	-6.74
2	3	1	4.21	3.46
3	3	1	9.69	-8.91
4	3	1	4.13	-4.01
5	3	1	0.30	-0.34
6	3	1	1.92	-1.25
7	3	1	1.61	-1.40
8	3	1	4.32	3.97
9	3	1	2.47	-2.23
10	3	1	0.53	0.50
11	3	1	0.33	0.19
12	3	1	3.38	-2.60
0	4	1	13.70	18.98
1	4	1	5.56	-5.03
2	4	1	1.04	-0.75
3	4	1	6.32	-5.55
4	4	1	0.52	-0.43
5	4	1	1.72	1.64
6	4	1	1.29	-1.30
7	4	1	5.58	-4.94
8	4	1	2.42	2.32
9	4	1	1.30	-1.11
10	4	1	0.64	-0.67
11	4	1	1.08	1.06
12	4	1	2.32	1.90
1	5	1	1.21	1.05
2	5	1	4.16	4.25
3	5	1	0.41	-0.05
4	5	1	5.18	4.77
5	5	1	4.06	-3.69
6	5	1	0.75	0.77
7	5	1	0.86	-0.65
8	5	1	1.95	-1.77
9	5	1	1.38	-1.57
10	5	1	0.94	-0.70
11	5	1	3.63	-3.28
12	5	1	0.42	-0.18
0	6	1	4.23	4.24
1	6	1	2.19	1.99
2	6	1	7.12	7.10
3	6	1	0.46	-0.46
4	6	1	8.07	7.16
5	6	1	5.13	-5.01
6	6	1	7.78	7.40
7	6	1	1.10	-1.12
8	6	1	6.08	5.24
9	6	1	0.75	-0.67
10	6	1	1.95	1.69
11	6	1	2.65	-2.57
1	7	1	10.29	9.90
2	7	1	2.41	-2.51
3	7	1	1.67	1.62
4	7	1	2.14	1.94
5	7	1	4.44	4.09
6	7	1	4.73	4.34
7	7	1	3.56	3.59
8	7	1	4.15	3.92
9	7	1	0.71	0.74
10	7	1	2.70	2.52
11	7	1	0.19	0.06
0	8	1	4.56	-3.93
1	8	1	1.90	1.60
2	8	1	2.00	1.91
3	8	1	2.66	2.35
4	8	1	1.61	-1.37
5	8	1	0.39	0.57
6	8	1	1.80	-1.97
7	8	1	2.49	2.33
8	8	1	4.54	-4.11
9	8	1	0.43	-0.14
10	8	1	1.41	1.26
1	9	1	1.35	-0.91
2	9	1	2.61	3.14
3	9	1	1.93	1.90
4	9	1	1.01	0.69
5	9	1	1.20	1.42
6	9	1	0.95	1.00
7	9	1	1.44	1.60
8	9	1	1.61	1.56
9	9	1	1.31	1.24
0	10	1	4.55	-4.19
1	10	1	1.79	-1.92
2	10	1	1.52	-1.79
3	10	1	0.67	0.56
4	10	1	5.03	-4.88
5	10	1	1.01	-1.03
6	10	1	2.23	-1.94
7	10	1	0.89	-0.74
8	10	1	3.98	-3.60
9	10	1	0.64	1.16
1	11	1	4.02	-3.69
2	11	1	0.36	-0.07
3	11	1	0.35	-0.41
4	11	1	0.75	0.76
5	11	1	1.75	-2.00
6	11	1	1.07	-1.13
7	11	1	4.53	-4.26
0	12	1	4.29	3.92
1	12	1	0.75	1.78
2	12	1	2.10	2.15
3	12	1	1.59	-1.43
4	12	1	2.88	2.55
5	12	1	1.84	-1.88
6	12	1	2.68	2.66
1	13	1	1.17	1.22
2	13	1	1.11	-1.16
3	13	1	0.21	-0.22
4	13	1	0.15	-0.56
0	0	2	0.88	-1.15
1	0	2	9.09	-9.97
2	0	2	7.04	-7.73
3	0	2	12.23	11.85
4	0	2	6.74	-6.25
5	0	2	1.16	1.44
6	0	2	5.45	5.43
7	0	2	7.46	6.75
8	0	2	7.81	-7.50
9	0	2	5.50	5.80
10	0	2	1.73	-1.96
11	0	2	0.45	0.58
12	0	2	3.75	-3.78
1	1	2	7.44	-7.63
2	1	2	2.23	2.08
3	1	2	11.46	-12.12
4	1	2	2.95	-2.70
5	1	2	3.19	2.95
6	1	2	3.56	3.58
7	1	2	11.71	-11.13
8	1	2	1.05	1.02
9	1	2	2.55	-2.53
10	1	2	1.90	2.16
11	1	2	0.51	-0.69
12	1	2	2.05	-2.22
0	2	2	7.73	-7.68
1	2	2	6.43	6.72
2	2	2	3.63	3.33
3	2	2	0.74	0.53
4	2	2	8.98	-8.45
5	2	2	1.52	1.58
6	2	2	2.49	-2.45
7	2	2	3.32	3.85
8	2	2	2.73	3.02
9	2	2	2.28	-2.35
10	2	2	0.28	0.66
11	2	2	4.04	4.44
12	2	2	2.04	2.30
1	3	2	10.96	-10.43
2	3	2	8.35	7.49
3	3	2	5.80	4.89
4	3	2	2.95	2.70
5	3	2	10.64	-10.10
6	3	2	5.03	-5.16
7	3	2	0.28	-0.68
8	3	2	2.60	2.36
9	3	2	3.71	-4.34
10	3	2	1.48	-1.16
11	3	2	2.04	-2.21
12	3	2	1.63	-1.85
0	4	2	0.53	0.38
1	4	2	3.47	-3.52
2	4	2	7.64	-6.86
3	4	2	3.91	3.77
4	4	2	4.12	4.67
5	4	2	0.56	-0.66
6	4	2	1.92	2.24
7	4	2	4.45	-4.11
8	4	2	2.57	2.54
9	4	2	3.27	3.50
10	4	2	3.89	4.01
11	4	2	4.95	-5.27
12	4	2	0.93	0.93
1	5	2	11.97	12.13
2	5	2	0.45	0.16
3	5	2	1.47	1.28
4	5	2	5.43	-5.32
5	5	2	10.32	10.31
6	5	2	2.29	2.40
7	5	2	2.00	2.18
8	5	2	2.32	-1.20
9	5	2	5.83	5.61
10	5	2	0.60	0.86
11	5	2	1.70	1.76
12	5	2	2.00	2.42
0	6	2	4.04	-3.76
1	6	2	7.14	7.38
2	6	2	1.27	0.00
3	6	2	5.58	-5.53
4	6	2	2.64	2.95
5	6	2	6.35	6.28
6	6	2	3.31	-3.72
7	6	2	3.97	3.88
8	6	2	0.69	-0.79
9	6	2	1.57	-1.89
10	6	2	3.31	-2.97
11	6	2	3.09	3.13
1	7	2	3.02	3.26
2	7	2	4.26	-4.08
3	7	2	6.21	6.17
4	7	2	5.78	5.81
5	7	2	0.71	-0.73
6	7	2	0.84	0.83
7	7	2	5.20	5.94
8	7	2	2.19	2.34
9	7	2	0.63	-0.58
10	7	2	1.47	1.39
11	7	2	1.61	1.52
0	8	2	0.48	-1.04
1	8	2	5.01	-5.09
2	8	2	4.83	-4.84
3	8	2	4.43	4.14
4	8	2	1.86	-1.46
5	8	2	3.91	4.07
6	8	2	4.11	-4.65
7	8	2	0.48	-0.13
8	8	2	1.75	-1.85
9	8	2	5.83	5.31
10	8	2	1.27	1.54
1	9	2	4.29	-4.49
2	9	2	3.19	3.87
3	9	2	5.54	-6.04
4	9	2	0.20	-0.50
5	9	2	0.65	-0.78
6	9	2	1.86	2.16
7	9	2	7.74	-7.64
8	9	2	1.88	-1.76
9	9	2	1.70	-1.71
0	10	2	2.92	-2.85
1	10	2	4.72	5.19
2	10	2	0.29	-0.07
3	10	2	0.76	-0.81
4	10	2	2.43	-2.43
5	10	2	2.52	-2.53
6	10	2	4.06	4.02
7	10	2	1.91	2.07
8	10	2	2.77	2.78
1	11	2	0.38	-0.15
2	11	2	2.94	-3.76
3	11	2	0.98	0.67
4	11	2	0.43	0.05
5	11	2	3.59	-3.93
6	11	2	1.50	-1.43
7	11	2	1.93	2.19
0	12	2	3.86	4.32
1	12	2	3.42	-3.82
2	12	2	1.65	1.82
3	12	2	2.20	2.27
4	12	2	2.15	0.29
5	12	2	1.05	-1.05
1	13	2	5.82	5.42
2	13	2	2.64	2.47
3	13	2	2.28	2.49
1	1	3	14.26	-14.87
2	1	3	6.89	-5.74
3	1	3	2.27	-2.43
4	1	3	1.54	1.11
5	1	3	6.49	-6.32
6	1	3	1.60	1.39
7	1	3	8.42	-8.90
8	1	3	0.80	-0.75
9	1	3	3.67	-3.95
10	1	3	1.11	0.71
11	1	3	1.21	-1.09
12	1	3	0.22	0.58
0	2	3	3.57	-3.40
1	2	3	1.22	-0.72
2	2	3	1.67	1.36
3	2	3	8.53	7.36
4	2	3	5.90	-6.01
5	2	3	3.06	-2.95
6	2	3	3.18	-3.15
7	2	3	1.60	1.66
8	2	3	0.76	-0.80
9	2	3	2.57	-2.88
10	2	3	0.32	-0.02
11	2	3	2.63	-2.30
12	2	3	1.11	-1.05
1	3	3	1.44	2.17
2	3	3	5.88	5.89
3	3	3	4.30	-4.90
4	3	3	1.63	-1.69
5	3	3	3.97	4.20
6	3	3	2.54	-2.46
7	3	3	9.84	9.51
8	3	3	1.15	-0.98
9	3	3	5.25	5.31
10	3	3	2.81	-2.63
11	3	3	3.98	3.82
12	3	3	0.47	-0.35
0	4	3	1.57	1.50
1	4	3	10.96	-10.38
2	4	3	2.29	-2.60
3	4	3	1.57	-1.21
4	4	3	1.12	-1.38
5	4	3	0.78	1.07
6	4	3	6.64	6.46
7	4	3	1.27	0.86
8	4	3	1.12	-0.87
9	4	3	2.23	-2.24
10	4	3	1.12	-1.19
11	4	3	2.84	2.95
12	4	3	0.33	-0.50
1	5	3	3.32	3.24
2	5	3	3.56	-3.79
3	5	3	1.47	1.39
4	5	3	2.33	-2.19
5	5	3	1.37	1.15
6	5	3	1.31	-0.47
7	5	3	3.50	2.99
8	5	3	0.54	0.19
9	5	3	2.42	2.57
10	5	3	1.27	1.44
11	5	3	1.83	1.81
0	6	3	1.35	1.42
1	6	3	0.94	1.19
2	6	3	4.49	4.51
3	6	3	1.22	1.10
4	6	3	1.37	0.96
5	6	3	2.99	2.57
6	6	3	2.41	-2.32
7	6	3	2.66	3.00
8	6	3	1.75	1.51
9	6	3	2.36	2.34
10	6	3	1.57	1.88
11	6	3	2.75	2.51
1	7	3	7.50	-7.73
2	7	3	3.36	3.16
3	7	3	5.73	-5.87
4	7	3	1.53	1.47
5	7	3	5.75	-5.53
6	7	3	0.82	-1.08
7	7	3	5.66	-5.99
8	7	3	0.30	0.31
9	7	3	4.28	-4.61
10	7	3	0.78	-0.49
0	8	3	2.13	-2.22
1	8	3	5.58	5.90
2	8	3	2.83	-2.99
3	8	3	1.91	1.91
4	8	3	1.86	1.86
5	8	3	0.58	0.44
6	8	3	0.75	-0.59
7	8	3	0.30	0.09
8	8	3	0.28	-0.22
9	8	3	3.44	3.18
10	8	3	0.16	0.03
1	9	3	4.88	-4.59
2	9	3	0.48	-0.14
3	9	3	4.48	-5.27
4	9	3	1.70	-1.92
5	9	3	2.54	-2.54
6	9	3	0.70	0.72
7	9	3	0.27	-0.15
8	9	3	0.24	-0.06
9	9	3	0.37	-0.07
0	10	3	1.20	-1.00
1	10	3	0.57	0.32
2	10	3	1.42	-1.50
3	10	3	1.95	-2.05
4	10	3	1.24	-1.27
5	10	3	0.30	-0.12
6	10	3	1.11	-1.03
7	10	3	2.31	-2.29
8	10	3	0.56	-0.64
1	11	3	3.48	3.75
2	11	3	2.35	-2.66
3	11	3	4.40	4.86
4	11	3	1.28	1.25
5	11	3	3.75	3.50
6	11	3	0.65	-0.75
7	11	3	2.73	3.10
0	12	3	1.54	1.21
1	12	3	1.06	-0.86
2	12	3	0.42	0.60
3	12	3	0.22	0.19
4	12	3	0.20	0.49
5	12	3	2.15	1.82
1	13	3	0.17	0.20
2	13	3	1.59	1.68
3	13	3	1.24	1.56
0	0	4	1.84	-1.78
1	0	4	9.41	8.92
2	0	4	1.45	1.03
3	0	4	1.52	0.80
4	0	4	10.20	-9.87
5	0	4	8.56	-8.70
6	0	4	9.78	-9.35
7	0	4	6.12	-6.60
8	0	4	4.57	-4.59
9	0	4	3.68	3.83
10	0	4	6.32	-6.01
11	0	4	8.16	-8.69
12	0	4	0.21	-0.38
1	1	4	8.94	8.27
2	1	4	7.08	6.70
3	1	4	7.25	-6.55
4	1	4	8.53	7.68
5	1	4	10.14	10.57
6	1	4	4.24	-4.65
7	1	4	1.84	1.51
8	1	4	0.35	0.70
9	1	4	3.39	3.14
10	1	4	2.29	-2.39
11	1	4	2.32	2.15
12	1	4	3.10	-3.12
0	2	4	0.56	0.24
1	2	4	4.57	4.26
2	2	4	8.64	-7.60
3	2	4	8.64	-9.22
4	2	4	1.38	1.60
5	2	4	0.98	0.91
6	2	4	4.54	4.07
7	2	4	2.00	-2.27
8	2	4	0.35	0.25
9	2	4	3.71	-3.73
10	2	4	2.16	1.86
11	2	4	2.48	2.14
12	2	4	1.40	-1.55
1	3	4	1.28	-1.04
2	3	4	3.35	3.21
3	3	4	9.54	10.03
4	3	4	6.32	-6.67
5	3	4	3.58	-3.28
6	3	4	1.65	1.43
7	3	4	4.93	4.63
8	3	4	1.28	-0.70
9	3	4	1.38	1.47
10	3	4	0.33	0.07
11	3	4	1.38	1.60
12	3	4	1.67	-1.48
0	4	4	0.35	-0.21
1	4	4	12.24	-12.06
2	4	4	8.09	7.59
3	4	4	2.13	2.40
4	4	4	2.66	2.47
5	4	4	0.33	-0.18
6	4	4	3.87	3.64
7	4	4	1.28	-1.48
8	4	4	6.96	6.64
9	4	4	0.49	0.54
10	4	4	2.22	2.50
11	4	4	0.58	-0.51
1	5	4	5.85	-6.42
2	5	4	4.32	-4.26
3	5	4	4.85	-4.67
4	5	4	2.24	2.16
5	5	4	0.34	0.72
6	5	4	2.46	-2.51
7	5	4	8.76	-9.36
8	5	4	2.16	2.18
9	5	4	0.80	-0.46
10	5	4	1.05	1.07
11	5	4	0.76	-0.77
0	6	4	2.21	2.09
1	6	4	3.67	3.83
2	6	4	1.57	-1.61
3	6	4	1.10	-1.14
4	6	4	1.68	1.80
5	6	4	4.34	-4.93
6	6	4	2.81	-3.13
7	6	4	2.32	2.38
8	6	4	4.90	-4.96
9	6	4	4.42	-5.00
10	6	4	0.98	1.16
11	6	4	1.50	1.49
1	7	4	2.77	-2.63
2	7	4	3.92	3.73
3	7	4	3.53	-3.64
4	7	4	0.88	0.87
5	7	4	5.50	-5.45
6	7	4	4.35	4.49
7	7	4	3.70	3.77
8	7	4	1.05	-1.07
9	7	4	3.33	-3.42
10	7	4	0.76	0.83
0	8	4	10.15	-10.53
1	8	4	7.01	-7.29
2	8	4	3.45	-3.44
3	8	4	1.17	1.37
4	8	4	3.87	-4.33
5	8	4	2.12	-2.12
6	8	4	2.60	-2.97
7	8	4	4.19	-4.37
8	8	4	1.16	-1.24
9	8	4	0.22	-0.20
1	9	4	4.30	4.32
2	9	4	3.08	-3.09
3	9	4	0.83	-0.55
4	9	4	1.04	0.81
5	9	4	4.42	4.51
6	9	4	2.25	-2.28
7	9	4	1.17	1.20
8	9	4	1.07	1.06
9	9	4	3.60	4.22
0	10	4	6.00	5.91
1	10	4	4.38	4.36
2	10	4	1.25	-0.89
3	10	4	3.58	-3.55
4	10	4	0.13	-0.02
5	10	4	0.30	0.31
6	10	4	1.64	1.73
7	10	4	0.66	0.67
8	10	4	1.53	1.29
1	11	4	1.62	-1.50
2	11	4	1.10	0.74
3	11	4	3.01	3.05
4	11	4	1.74	-1.79
5	11	4	1.57	-1.52
6	11	4	0.78	0.70
0	12	4	1.67	1.41
1	12	4	0.25	-0.37
2	12	4	4.14	4.50
3	12	4	0.83	1.05
4	12	4	2.48	2.71
1	13	4	3.17	-3.12
1	1	5	6.16	5.85
2	1	5	2.36	-2.18
3	1	5	3.73	3.94
4	1	5	0.26	-0.01
5	1	5	1.95	1.93
6	1	5	3.02	-2.73
7	1	5	0.14	0.02
8	1	5	3.89	-4.19
9	1	5	0.78	-0.95
10	1	5	2.47	-2.29
11	1	5	1.12	-0.95
12	1	5	2.15	-2.06
0	2	5	7.71	7.19
1	2	5	0.78	0.65
2	2	5	7.97	7.34
3	2	5	2.74	-2.52
4	2	5	4.12	3.63
5	2	5	7.53	7.61
6	2	5	8.73	9.22
7	2	5	0.34	-0.29
8	2	5	7.94	7.91
9	2	5	0.47	0.39
10	2	5	3.33	3.00
11	2	5	0.82	-0.35
12	2	5	1.47	1.69
1	3	5	3.11	-2.55
2	3	5	3.69	-3.25
3	3	5	2.11	2.01
4	3	5	4.34	-3.98
5	3	5	0.32	-0.27
6	3	5	1.43	1.50
7	3	5	0.49	-0.37
8	3	5	2.73	2.39
9	3	5	1.28	1.03
10	3	5	0.66	0.48
11	3	5	0.90	0.66
0	4	5	5.29	4.30
1	4	5	2.50	2.40
2	4	5	1.16	-1.04
3	4	5	3.81	-3.65
4	4	5	5.25	-4.80
5	4	5	1.26	-1.14
6	4	5	0.75	-0.67
7	4	5	3.02	-3.16
8	4	5	3.63	-3.13
9	4	5	0.32	0.49
10	4	5	0.26	-0.12
11	4	5	1.34	-1.19
1	5	5	3.93	3.69
2	5	5	2.96	2.88
3	5	5	0.90	-0.69
4	5	5	2.09	2.16
5	5	5	1.62	1.54
6	5	5	0.00	-1.24
7	5	5	0.49	0.31
8	5	5	1.42	-1.23
9	5	5	1.63	-1.45
10	5	5	1.55	1.08
11	5	5	1.46	-1.57
0	6	5	12.35	-13.45
1	6	5	0.32	0.08
2	6	5	6.80	-6.81
3	6	5	1.10	-1.24
4	6	5	3.62	-3.21
5	6	5	1.65	-1.89
6	6	5	5.46	-5.79
7	6	5	0.82	-0.81
8	6	5	3.93	-4.16
9	6	5	0.47	-0.47
10	6	5	3.47	-3.43
1	7	5	4.43	4.78
2	7	5	0.82	0.74
3	7	5	1.99	1.87
4	7	5	4.06	-4.16
5	7	5	0.34	-0.12
6	7	5	3.66	-3.83
7	7	5	1.09	1.21
8	7	5	0.28	0.17
9	7	5	0.82	-0.74
10	7	5	1.40	-1.60
0	8	5	3.00	3.27
1	8	5	1.75	-2.01
2	8	5	1.00	0.87
3	8	5	2.82	2.98
4	8	5	1.42	1.21
5	8	5	0.34	-0.15
6	8	5	0.64	0.58
7	8	5	1.67	1.29
8	8	5	2.44	2.30
9	8	5	1.35	-0.97
1	9	5	0.84	-0.90
2	9	5	1.53	-1.26
3	9	5	0.67	0.69
4	9	5	1.38	-1.17
5	9	5	1.48	1.50
6	9	5	0.28	-0.27
7	9	5	0.24	-0.26
8	9	5	2.39	-2.28
0	10	5	4.00	4.51
1	10	5	0.32	-0.12
2	10	5	3.62	3.81
3	10	5	0.30	-0.42
4	10	5	3.98	4.35
5	10	5	2.72	-2.69
6	10	5	3.75	3.59
7	10	5	0.36	0.19
1	11	5	0.28	-0.26
2	11	5	1.77	-1.68
3	11	5	1.15	1.00
4	11	5	2.63	2.54
5	11	5	0.20	-0.46
6	11	5	1.19	1.41
0	12	5	4.16	-4.62
1	12	5	0.99	-0.90
2	12	5	3.10	-2.67
3	12	5	0.94	-0.52
4	12	5	1.46	-1.23
0	0	6	9.53	8.29
1	0	6	3.07	2.87
2	0	6	13.21	14.47
3	0	6	3.29	3.18
4	0	6	6.61	7.37
5	0	6	4.30	-4.72
6	0	6	4.81	5.27
7	0	6	3.29	3.69
8	0	6	10.14	9.54
9	0	6	1.00	-0.51
10	0	6	4.26	-4.35
11	0	6	1.17	-0.90
1	1	6	2.54	2.54
2	1	6	5.08	-4.93
3	1	6	2.13	2.03
4	1	6	6.09	5.95
5	1	6	2.32	2.17
6	1	6	0.90	-0.37
7	1	6	2.39	2.24
8	1	6	7.01	6.72
9	1	6	1.37	1.12
10	1	6	0.30	0.37
11	1	6	2.66	2.52
0	2	6	13.02	12.11
1	2	6	2.02	-1.91.
2	2	6	5.28	-4.97
3	2	6	2.62	3.01
4	2	6	2.25	2.60
5	2	6	0.35	0.16
6	2	6	0.53	-0.24
7	2	6	0.38	0.08
8	2	6	3.86	-3.49
9	2	6	0.80	0.73
10	2	6	3.38	3.21
11	2	6	0.98	0.78
1	3	6	0.67	0.08
2	3	6	4.95	4.80
3	3	6	4.74	4.69
4	3	6	2.99	-3.01
5	3	6	2.72	2.82
6	3	6	5.65	5.47
7	3	6	0.54	-0.27
8	3	6	2.66	-2.87
9	3	6	2.32	2.05
10	3	6	1.35	1.35
11	3	6	1.03	1.36
0	4	6	16.08	-16.37
1	4	6	0.81	0.67
2	4	6	1.05	0.78
3	4	6	1.53	-1.47
4	4	6	4.97	-5.08
5	4	6	2.92	3.25
6	4	6	4.57	-4.78
7	4	6	0.97	1.02
8	4	6	2.42	-2.32
9	4	6	1.61	1.25
10	4	6	5.09	-5.09
11	4	6	2.17	1.75
1	5	6	2.66	-2.49
2	5	6	2.73	-3.23
3	5	6	0.35	-0.31
4	5	6	1.00	0.74
5	5	6	3.07	-3.07
6	5	6	9.17	-9.60
7	5	6	2.57	-2.39
8	5	6	0.80	0.55
9	5	6	1.91	-1.92
10	5	6	1.60	-1.66
0	6	6	9.42	9.39
1	6	6	0.89	0.94
2	6	6	2.50	2.07
3	6	6	1.29	-1.06
4	6	6	3.07	3.17
5	6	6	2.45	2.77
6	6	6	3.16	3.26
7	6	6	0.35	0.10
8	6	6	2.19	-2.17
9	6	6	1.13	0.67
10	6	6	2.06	2.13
1	7	6	0.78	0.59
2	7	6	1.61	1.50
3	7	6	3.87	-3.92
4	7	6	4.90	-5.09
5	7	6	0.38	-0.25
6	7	6	4.38	4.33
7	7	6	0.33	-0.03
8	7	6	2.54	-2.55
9	7	6	1.45	-1.27
0	8	6	3.45	3.62
1	8	6	0.38	-0.08
2	8	6	8.87	9.50
3	8	6	0.67	-0.65
4	8	6	2.03	1.78
5	8	6	1.02	1.23
6	8	6	3.55	3.83
7	8	6	1.68	-1.47
8	8	6	5.01	4.73
1	9	6	2.39	2.40
2	9	6	2.50	-2.64
3	9	6	2.57	2.93
4	9	6	5.16	6.10
5	9	6	1.87	1.66
6	9	6	1.75	-1.38
7	9	6	3.33	2.67
0	10	6	0.92	-1.09
1	10	6	0.33	0.15
2	10	6	4.95	-5.39
3	10	6	1.20	1.00
4	10	6	2.07	2.05
5	10	6	1.98	-1.52
6	10	6	1.16	-0.93
1	11	6	2.07	1.80
2	11	6	1.16	1.22
3	11	6	0.94	0.57
4	11	6	5.67	-5.32
5	11	6	0.90	0.87
0	12	6	1.59	-2.10
1	12	6	0.53	0.47
1	1	7	7.70	6.83
2	1	7	3.16	-2.84
3	1	7	3.73	3.44
4	1	7	3.85	3.87
5	1	7	3.92	3.80
6	1	7	4.70	4.89
7	1	7	2.91	3.08
8	1	7	1.20	1.20
9	1	7	1.17	1.63
10	1	7	1.61	1.60
11	1	7	1.44	1.53
0	2	7	2.01	-0.97
1	2	7	2.57	-2.18
2	2	7	5.01	-4.77
3	2	7	3.37	3.39
4	2	7	1.53	-1.28
5	2	7	5.01	4.90
6	2	7	4.73	-5.16
7	2	7	3.22	2.76
8	2	7	1.36	-1.09
9	2	7	0.91	0.89
10	2	7	1.32	-1.43
1	3	7	8.79	-9.73
2	3	7	4.95	5.45
3	3	7	3.11	-2.90
4	3	7	0.30	-0.23
5	3	7	4.43	-4.50
6	3	7	1.83	-1.30
7	3	7	3.79	-3.62
8	3	7	0.75	0.73
9	3	7	1.01	-1.00
10	3	7	0.30	-0.09
0	4	7	5.84	5.53
1	4	7	0.41	0.04
2	4	7	1.99	-1.70
3	4	7	1.16	-0.84
4	4	7	0.86	0.87
5	4	7	4.23	-4.41
6	4	7	2.62	2.68
7	4	7	0.44	0.47
8	4	7	2.19	2.13
9	4	7	0.24	-0.20
10	4	7	3.16	-3.12
1	5	7	0.61	-0.62
2	5	7	0.63	-0.37
3	5	7	4.49	-4.65
4	5	7	0.33	0.17
5	5	7	2.28	-2.12
6	5	7	0.76	0.41
7	5	7	2.68	-2.34
8	5	7	2.57	2.49
9	5	7	3.36	-2.87
10	5	7	1.03	1.35
0	6	7	4.65	5.59
1	6	7	0.31	-0.15
2	6	7	4.28	4.46
3	6	7	1.03	-0.77
4	6	7	1.93	2.02
5	6	7	0.97	-1.00
6	6	7	1.03	0.92
7	6	7	2.84	-2.63
8	6	7	1.88	1.57
9	6	7	2.17	-2.01
1	7	7	5.42	5.59
2	7	7	2.32	2.18
3	7	7	4.70	5.20
4	7	7	2.81	2.49
5	7	7	3.01	3.44
6	7	7	2.45	2.75
7	7	7	3.97	4.00
8	7	7	0.93	0.90
0	8	7	6.21	-5.92
1	8	7	0.31	-0.04
2	8	7	1.27	1.23
3	8	7	0.86	0.60
4	8	7	1.31	1.04
5	8	7	2.45	2.65
6	8	7	0.25	-0.14
7	8	7	1.08	0.93
8	8	7	1.75	-1.92
1	9	7	0.10	0.03
2	9	7	0.28	0.33
3	9	7	1.06	1.38
4	9	7	0.25	0.21
5	9	7	2.02	1.70
6	9	7	0.19	0.03
7	9	7	0.75	0.75
0	10	7	1.09	-0.88
1	10	7	1.73	1.69
2	10	7	0.24	-0.51
3	10	7	0.96	-0.60
4	10	7	1.83	-1.73
5	10	7	0.16	-0.04
1	11	7	3.73	-3.43
2	11	7	1.08	-0.62
3	11	7	3.13	-3.62
0	0	8	5.33	-5.05
1	0	8	6.10	6.66
2	0	8	5.30	6.80
3	0	8	0.22	-0.26
4	0	8	1.65	-1.52
5	0	8	3.78	3.91
6	0	8	3.07	-2.67
7	0	8	5.18	4.91
8	0	8	1.24	-1.00
9	0	8	0.90	-0.28
10	0	8	2.06	1.74
1	1	8	8.38	-9.48
2	1	8	4.03	4.62
3	1	8	0.84	0.87
4	1	8	2.88	2.94
5	1	8	7.60	-7.21
6	1	8	1.21	-0.80
7	1	8	1.29	-1.45
8	1	8	2.34	1.99
9	1	8	4.85	-3.91
10	1	8	1.05	-1.01
0	2	8	1.44	-2.09
1	2	8	3.52	-3.91
2	2	8	4.21	-4.74
3	2	8	2.52	3.07
4	2	8	1.83	-1.78
5	2	8	1.70	-1.37
6	2	8	3.53	3.11
7	2	8	1.57	-1.32
8	2	8	1.17	-0.90
9	2	8	4.41	3.84
10	2	8	1.28	1.31
1	3	8	3.46	-3.45
2	3	8	0.22	-0.16
3	3	8	4.34	-5.04
4	3	8	1.47	-1.27
5	3	8	1.05	0.81
6	3	8	1.98	2.15
7	3	8	7.65	-7.49
8	3	8	0.22	-0.08
9	3	8	1.36	-0.57
10	3	8	1.21	1.32
0	4	8	2.58	-2.82
1	4	8	3.07	4.20
2	4	8	2.52	-2.86
3	4	8	2.69	-3.21
4	4	8	2.69	-2.85
5	4	8	1.34	-1.16
6	4	8	1.94	-1.76
7	4	8	0.22	-0.26
8	4	8	2.27	1.95
9	4	8	4.83	-3.98
1	5	8	5.69	5.71
2	5	8	2.80	-3.31
3	5	8	7.41	7.66
4	5	8	1.16	1.20
5	5	8	0.57	0.46
6	5	8	1.60	-1.43
7	5	8	7.75	7.15
8	5	8	0.84	-0.45
9	5	8	1.85	1.43
0	6	8	1.91	2.10
1	6	8	4.72	-5.40
2	6	8	1.72	-1.77
3	6	8	2.82	2.79
4	6	8	2.49	2.57
5	6	8	2.95	3.18
6	6	8	2.93	-3.06
7	6	8	0.19	0.13
8	6	8	0.96	-0.40
1	7	8	2.97	3.32
2	7	8	3.42	3.98
3	7	8	1.16	-0.87
4	7	8	0.60	-0.45
5	7	8	6.22	5.67
6	7	8	1.91	1.90
7	7	8	0.16	-0.04
0	8	8	1.87	-1.42
1	8	8	2.50	2.97
2	8	8	1.01	-1.09
3	8	8	1.49	-1.52
4	8	8	0.12	-0.07
5	8	8	2.21	1.88
6	8	8	1.61	1.47
7	8	8	2.62	2.08
1	9	8	4.51	-4.82
2	9	8	1.59	-1.31
3	9	8	2.15	-1.79
4	9	8	1.78	1.78
5	9	8	6.83	-6.54
0	10	8	0.84	-0.48
1	10	8	1.09	-1.09
2	10	8	1.21	-1.12
3	10	8	2.87	2.28
4	10	8	1.95	-1.88
1	1	9	3.19	-4.06
2	1	9	0.91	-0.54
3	1	9	2.81	-3.58
4	1	9	1.23	1.06
5	1	9	2.14	-2.59
6	1	9	1.23	0.70
7	1	9	2.30	-2.08
8	1	9	0.80	-0.30
9	1	9	2.33	-2.48
0	2	9	3.37	-5.66
1	2	9	1.03	0.32
2	2	9	4.22	-4.44
3	2	9	1.38	1.60
4	2	9	4.79	-5.08
5	2	9	1.16	-1.18
6	2	9	0.25	-0.21
7	2	9	0.05	-0.75
8	2	9	3.77	-4.79
9	2	9	0.13	0.14
1	3	9	1.47	1.43
2	3	9	2.03	-2.56
3	3	9	1.83	1.20
4	3	9	3.03	-3.07
5	3	9	1.24	1.03
6	3	9	2.03	-2.04
7	3	9	4.17	3.70
8	3	9	1.89	-1.57
9	3	9	3.90	4.19
0	4	9	1.46	1.41
1	4	9	1.22	0.30
2	4	9	2.61	3.11
3	4	9	0.26	-0.11
4	4	9	1.03	-1.05
5	4	9	1.22	-1.03
6	4	9	0.41	0.31
7	4	9	1.28	0.92
8	4	9	0.62	-0.20
1	5	9	1.36	1.20
2	5	9	2.45	2.07
3	5	9	0.71	0.70
4	5	9	0.25	-0.37
5	5	9	2.09	2.26
6	5	9	2.14	-2.21
7	5	9	2.81	1.72
8	5	9	1.24	-1.10
0	6	9	2.33	2.14
1	6	9	1.68	-1.53
2	6	9	1.96	1.99
3	6	9	0.25	-0.15
4	6	9	3.65	4.05
5	6	9	2.60	2.34
6	6	9	4.25	3.55
7	6	9	1.24	1.13
1	7	9	3.72	-4.26
2	7	9	0.47	0.28
3	7	9	1.70	-1.88
4	7	9	0.82	-0.82
5	7	9	3.90	-3.33
6	7	9	1.27	0.84
0	8	9	2.77	-1.95
1	8	9	1.80	1.69
2	8	9	2.24	-2.10
3	8	9	1.72	1.37
4	8	9	0.67	-0.49
5	8	9	1.17	0.57
1	9	9	2.76	-2.45
2	9	9	1.27	-0.94
3	9	9	2.92	-2.54
0	0	10	4.29	-3.87
0	2	10	3.34	0.12
0	4	10	7.63	7.09
0	6	10	4.13	-4.25
0	8	10	0.83	-0.86
0	2	11	8.40	7.85
0	4	11	2.18	-2.18
0	6	11	2.69	-3.05
0	0	12	8.20	8.60
0	2	12	4.92	-4.37
0	4	12	0.79	0.48

Table 3. *Distances and angles within the phosphate tetrahedron and magnesium octahedron*

See Table 4 for key to superscripts.

Phosphate tetrahedron

P–O(3)	1·500 Å
P–O(4)	1·542
P–O(5)	1·545
P–O(6)	1·588

	O···O	∠O–P–O
O(3)···O(4)	2·546 Å	113·4°
O(3)···O(5)	2·550	113·5
O(3)···O(6)	2·466	105·6
O(4)···O(5)	2·516	109·1
O(4)···O(6)	2·522	107·2
O(5)···O(6)	2·509	106·3

Magnesium octahedron

Mg–O(3′)	2·021 Å
Mg–O(4″)	2·073
Mg–O(5)	2·053
Mg–O(7)	2·107
Mg–O(8)	2·121
Mg–O(9)	2·127

	O···O	∠O–Mg–O
O(3′)···O(4″)	2·951 Å	92·2°
O(3′)···O(5)	2·918	91·3
O(3′)···O(8)	2·877	87·6
O(3′)···O(9)	3·055	94·5
O(4″)···O(7)	2·941	89·3
O(4″)···O(8)	2·960	89·5
O(4″)···O(9)	2·816	84·1
O(5)···O(7)	2·866	87·0
O(5)···O(8)	3·007	92·1
O(5)···O(9)	3·048	93·4
O(7)···O(8)	2·848	84·4
O(7)···O(9)	3·062	92·4

Secondly, variations in bond lengths of 2·046–2·108 Å were observed in struvite, where magnesium is coordinated by water molecules only. Nevertheless, this division of Mg–O distances in newberyite is in accordance with a greater ionic character, resulting from the interaction of the ions Mg^{2+} and HPO_4^{2-}, for the bonds in group (2).

Angles within the octahedron deviate considerably from a right angle. This is apparently the case in most compounds containing this group.

The sharing of phosphate oxygen atoms with magnesium atoms results in a close-packed structure. The O···O intermolecular contacts less than 3·21 Å are given in Table 4 and O···O distances in the octahedron in Table 3. As mentioned previously, the shortest of these O(4)···O(6) represents a hydrogen bond, and it is reasonable to assume that O(7) and O(8) act as donor atoms in two hydrogen bonds O(7)···O(5) of 2·762 Å and O(8)···O(6) of 2·684 Å. The next four shortest distances in Table 4 could be the remaining hydrogen bonds, and this solution gives an acceptable arrangement around all atoms involved. There is, however, the possibility of hydrogen bonding within the magnesium octahedron and the unequivocal assignment of the last four hydrogen atoms to definite O···O distances is not possible here.

The crystal structure can broadly be described as alternate planes of magnesium and phosphorus atoms parallel to (100), separated by approximately $\frac{1}{4}x$ and linked by the sharing of oxygen atoms and hydrogen bonds (Fig. 1). Arrangement of atoms within the planes is such that magnesium and phosphorus also lie on planes parallel to (010). Each of these magnesium planes is sandwiched by two different planes of phosphorus atoms providing oxygen atoms for the octahedral coordination. Hydrogen bonds hold the planes together, and the breaking of these, between adjacent phosphorus planes, corresponds to the perfect (010) cleavage.

Table 4. O···O *contacts less than* 3·21 Å

See Table 3 for O···O distances in the octahedron.

Atoms in equivalent positions are represented by the superscripts:

′	$\frac{1}{2}+x,\ y,\ \frac{1}{2}-z$
″	$\frac{1}{2}+x,\ \frac{1}{2}-y,\ \bar{z}$
‴	$\bar{x},\ \bar{y},\ \bar{z}$
iv	$\bar{x},\ \frac{1}{2}+y,\ \frac{1}{2}-z$
v	$x,\ \frac{1}{2}-y,\ \frac{1}{2}+z$
vi	$\frac{1}{2}-x,\ \frac{1}{2}+y,\ z$

O(4)···O(6‴)	2·609 Å	O(7)···O(9^{vi})	2·993 Å
O(8)···O(6^{iv})	2·684	O(8)···O(6^{vi})	3·015
O(5)···O(7^{v})	2·762	O(8)···O(9^{vi})	3·114
O(8)···O(5^{vi})	2·804	O(7)···O(3″)	3·183
O(4)···O(7)	2·843	O(3)···O(7^{v})	3·189
O(8)···O(9^{v})	2·984	O(9)···O(3″)	3·205

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