

Abstract**Table 1**

Experimental details

Crystal data	
Chemical formula	$\text{Ca}_{10}\text{H}_2\text{O}_{26}\text{P}_6$
M_r	1004.63
Crystal system, space group	Hexagonal, $P6_3/m$
Temperature (K)	300
a, c (Å)	9.3731 (4), 6.8769 (3)
V (Å ³)	523.23 (5)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	3.10
Crystal size (mm)	$0.07 \times 0.06 \times 0.05$
Data collection	
Diffractometer	Bruker D8 Venture Photon 100 CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause et al., 2015)
T_{\min}, T_{\max}	0.695, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26729, 438, 388
R_{int}	0.087
$(\sin \theta/\lambda)_{\max}$ (Å ⁻¹)	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.022, 0.049, 1.13
No. of reflections	438
No. of parameters	42
No. of restraints	7
H-atom treatment	All H-atom parameters refined
$(\Delta/\sigma)_{\max}$	3.238
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å ⁻³)	0.88, -0.50

Computer programs: *SHELXL2019/1* (Sheldrick, 2019).**References**

NOT FOUND

full crystallographic data

Computing details

Program(s) used to refine structure: *SHELXL2019/1* (Sheldrick, 2019).

(linhuishi_TB_jinghuashangmao_20230803_S1)

Crystal data

Ca ₁₀ H ₂ O ₂₆ P ₆	$D_x = 3.188 \text{ Mg m}^{-3}$
$M_r = 1004.63$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hexagonal, $P6_3/m$	Cell parameters from 8178 reflections
$a = 9.3731 (4) \text{ \AA}$	$\theta = 2.5\text{--}27.5^\circ$
$c = 6.8769 (3) \text{ \AA}$	$\mu = 3.10 \text{ mm}^{-1}$
$V = 523.23 (5) \text{ \AA}^3$	$T = 300 \text{ K}$
$Z = 1$	Lump, colourless
$F(000) = 500$	$0.07 \times 0.06 \times 0.05 \text{ mm}$

Data collection

Bruker D8 Venture Photon 100 CMOS diffractometer	438 independent reflections
phi and ω scans	388 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Krause et al., 2015)	$R_{\text{int}} = 0.087$
$T_{\text{min}} = 0.695$, $T_{\text{max}} = 0.746$	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.5^\circ$
26729 measured reflections	$h = -12 \rightarrow 12$
	$k = -12 \rightarrow 12$
	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 0.7283P]$
$wR(F^2) = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{\text{max}} = 3.238$
438 reflections	$\Delta\rho_{\text{max}} = 0.88 \text{ e \AA}^{-3}$
42 parameters	$\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$
7 restraints	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2) for
(linhuishi_TB_jinghuashangmao_20230803_S1)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ca1	0.666667	0.333333	0.00112 (11)	0.0094 (2)	
Ca2	−0.00720 (7)	0.24198 (8)	0.250000	0.00777 (17)	
P1	0.36889 (9)	0.39830 (9)	0.250000	0.00605 (19)	
O1	0.4847 (3)	0.3270 (3)	0.250000	0.0107 (5)	
O2	0.4668 (3)	0.5878 (3)	0.250000	0.0120 (5)	

O3	0.25715 (19)	0.3417 (2)	0.0706 (2)	0.0142 (4)	
O4	0.000000	0.000000	0.2700 (14)	0.0018 (9)	0.5
H1	0.000000	0.000000	0.155 (3)	0.00 (2)*	0.5

Atomic displacement parameters (\AA^2) for (linhuishi_TB_jinghuashangmao_20230803_S1)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0112 (3)	0.0112 (3)	0.0059 (4)	0.00558 (13)	0.000	0.000
Ca2	0.0072 (3)	0.0088 (3)	0.0071 (3)	0.0039 (2)	0.000	0.000
P1	0.0062 (4)	0.0069 (4)	0.0061 (4)	0.0040 (3)	0.000	0.000
O1	0.0105 (11)	0.0135 (11)	0.0117 (11)	0.0087 (9)	0.000	0.000
O2	0.0093 (11)	0.0076 (11)	0.0187 (12)	0.0040 (9)	0.000	0.000
O3	0.0124 (8)	0.0243 (9)	0.0091 (8)	0.0114 (7)	−0.0036 (7)	−0.0067 (7)
O4	0.0021 (9)	0.0021 (9)	0.0013 (15)	0.0010 (4)	0.000	0.000

Geometric parameters (\AA , $^\circ$) for (linhuishi_TB_jinghuashangmao_20230803_S1)

Ca1—O1 ⁱ	2.3957 (15)	Ca2—O2 ^{ix}	2.370 (2)
Ca1—O1 ⁱⁱ	2.3957 (15)	Ca2—O3	2.4940 (16)
Ca1—O1	2.3957 (15)	Ca2—O3 ^{vi}	2.4940 (16)
Ca1—O2 ⁱⁱⁱ	2.4530 (16)	Ca2—O1 ^x	2.691 (2)
Ca1—O2 ^{iv}	2.4530 (16)	Ca2—P1	3.0673 (10)
Ca1—O2 ^v	2.4530 (16)	Ca2—P1 ^x	3.2533 (10)
Ca1—O3 ^{iv}	2.8031 (17)	Ca2—P1 ^{ix}	3.4885 (10)
Ca1—O3 ⁱⁱⁱ	2.8031 (17)	Ca2—H1	2.394 (6)
Ca1—O3 ^v	2.8031 (17)	Ca2—H1 ^{vi}	2.394 (6)
Ca1—P1 ⁱⁱⁱ	3.2030 (7)	P1—O3 ^{vi}	1.5314 (17)
Ca1—P1 ^{iv}	3.2030 (7)	P1—O3	1.5314 (17)
Ca1—P1 ^v	3.2030 (7)	P1—O1	1.533 (2)
Ca2—O4	2.3067 (8)	P1—O2	1.539 (2)
Ca2—O4 ^{vi}	2.3067 (8)	O4—O4 ^{vi}	0.276 (19)
Ca2—O3 ^{vii}	2.3471 (16)	O4—H1	0.79 (2)
Ca2—O3 ^{viii}	2.3471 (16)	O4—H1 ^{vi}	0.52 (3)
O1 ⁱ —Ca1—O1 ⁱⁱ	74.60 (6)	O3 ^{vii} —Ca2—P1 ^{ix}	78.96 (4)
O1 ⁱ —Ca1—O1	74.60 (6)	O3 ^{viii} —Ca2—P1 ^{ix}	78.96 (4)
O1 ⁱⁱ —Ca1—O1	74.60 (6)	O2 ^{ix} —Ca2—P1 ^{ix}	21.17 (5)
O1 ⁱ —Ca1—O2 ⁱⁱⁱ	92.67 (5)	O3—Ca2—P1 ^{ix}	92.77 (4)
O1 ⁱⁱ —Ca1—O2 ⁱⁱⁱ	154.34 (7)	O3 ^{vi} —Ca2—P1 ^{ix}	92.77 (4)
O1—Ca1—O2 ⁱⁱⁱ	124.12 (7)	O1 ^x —Ca2—P1 ^{ix}	79.61 (5)
O1 ⁱ —Ca1—O2 ^{iv}	124.12 (7)	P1—Ca2—P1 ^{ix}	90.68 (3)
O1 ⁱⁱ —Ca1—O2 ^{iv}	92.67 (5)	P1 ^x —Ca2—P1 ^{ix}	107.51 (3)
O1—Ca1—O2 ^{iv}	154.34 (7)	O4—Ca2—Ca1 ^{xi}	130.16 (13)
O2 ⁱⁱⁱ —Ca1—O2 ^{iv}	75.91 (6)	O4 ^{vi} —Ca2—Ca1 ^{xi}	126.38 (14)
O1 ⁱ —Ca1—O2 ^v	154.34 (7)	O3 ^{vii} —Ca2—Ca1 ^{xi}	44.32 (4)
O1 ⁱⁱ —Ca1—O2 ^v	124.12 (7)	O3 ^{viii} —Ca2—Ca1 ^{xi}	95.62 (5)
O1—Ca1—O2 ^v	92.67 (5)	O2 ^{ix} —Ca2—Ca1 ^{xi}	75.66 (5)
O2 ⁱⁱⁱ —Ca1—O2 ^v	75.91 (6)	O3—Ca2—Ca1 ^{xi}	115.83 (4)
O2 ^{iv} —Ca1—O2 ^v	75.91 (6)	O3 ^{vi} —Ca2—Ca1 ^{xi}	149.78 (4)
O1 ⁱ —Ca1—O3 ^{iv}	68.97 (6)	O1 ^x —Ca2—Ca1 ^{xi}	36.38 (3)
O1 ⁱⁱ —Ca1—O3 ^{iv}	86.79 (6)	P1—Ca2—Ca1 ^{xi}	136.474 (19)

O1—Ca1—O3 ^{iv}	142.36 (6)	P1 ^x —Ca2—Ca1 ^{xi}	58.552 (15)
O2 ⁱⁱⁱ —Ca1—O3 ^{iv}	67.73 (6)	P1 ^{ix} —Ca2—Ca1 ^{xi}	57.040 (14)
O2 ^{iv} —Ca1—O3 ^{iv}	55.95 (6)	O4—Ca2—H1	19.3 (5)
O2 ^v —Ca1—O3 ^{iv}	124.57 (6)	O4 ^{vi} —Ca2—H1	12.4 (6)
O1 ⁱ —Ca1—O3 ⁱⁱⁱ	86.79 (6)	O3 ^{vii} —Ca2—H1	87.5 (5)
O1 ⁱⁱ —Ca1—O3 ⁱⁱⁱ	142.36 (6)	O3 ^{viii} —Ca2—H1	118.0 (5)
O1—Ca1—O3 ⁱⁱⁱ	68.97 (6)	O2 ^{ix} —Ca2—H1	148.6 (2)
O2 ⁱⁱⁱ —Ca1—O3 ⁱⁱⁱ	55.95 (6)	O3—Ca2—H1	74.1 (2)
O2 ^{iv} —Ca1—O3 ⁱⁱⁱ	124.57 (6)	O3 ^{vi} —Ca2—H1	89.8 (3)
O2 ^v —Ca1—O3 ⁱⁱⁱ	67.73 (6)	O1 ^x —Ca2—H1	106.08 (7)
O3 ^{iv} —Ca1—O3 ⁱⁱⁱ	116.97 (2)	P1—Ca2—H1	83.25 (3)
O1 ⁱ —Ca1—O3 ^v	142.36 (6)	P1 ^x —Ca2—H1	79.26 (4)
O1 ⁱⁱ —Ca1—O3 ^v	68.97 (6)	P1 ^{ix} —Ca2—H1	163.0 (5)
O1—Ca1—O3 ^v	86.79 (6)	Ca1 ^{xi} —Ca2—H1	118.6 (3)
O2 ⁱⁱⁱ —Ca1—O3 ^v	124.57 (6)	O4—Ca2—H1 ^{vi}	12.4 (6)
O2 ^{iv} —Ca1—O3 ^v	67.73 (6)	O4 ^{vi} —Ca2—H1 ^{vi}	19.3 (5)
O2 ^v —Ca1—O3 ^v	55.95 (6)	O3 ^{vii} —Ca2—H1 ^{vi}	118.0 (5)
O3 ^{iv} —Ca1—O3 ^v	116.97 (2)	O3 ^{viii} —Ca2—H1 ^{vi}	87.5 (5)
O3 ⁱⁱⁱ —Ca1—O3 ^v	116.97 (2)	O2 ^{ix} —Ca2—H1 ^{vi}	148.6 (2)
O1 ⁱ —Ca1—P1 ⁱⁱⁱ	93.00 (4)	O3—Ca2—H1 ^{vi}	89.8 (3)
O1 ⁱⁱ —Ca1—P1 ⁱⁱⁱ	166.60 (5)	O3 ^{vi} —Ca2—H1 ^{vi}	74.1 (2)
O1—Ca1—P1 ⁱⁱⁱ	97.50 (5)	O1 ^x —Ca2—H1 ^{vi}	106.08 (6)
O2 ⁱⁱⁱ —Ca1—P1 ⁱⁱⁱ	27.74 (5)	P1—Ca2—H1 ^{vi}	83.25 (3)
O2 ^{iv} —Ca1—P1 ⁱⁱⁱ	98.63 (5)	P1 ^x —Ca2—H1 ^{vi}	79.26 (4)
O2 ^v —Ca1—P1 ⁱⁱⁱ	66.19 (5)	P1 ^{ix} —Ca2—H1 ^{vi}	163.0 (5)
O3 ^{iv} —Ca1—P1 ⁱⁱⁱ	93.56 (4)	Ca1 ^{xi} —Ca2—H1 ^{vi}	135.62 (18)
O3 ⁱⁱⁱ —Ca1—P1 ⁱⁱⁱ	28.56 (3)	H1—Ca2—H1 ^{vi}	31.7 (10)
O3 ^v —Ca1—P1 ⁱⁱⁱ	122.12 (4)	O3 ^{vi} —P1—O3	107.36 (13)
O1 ⁱ —Ca1—P1 ^{iv}	97.50 (5)	O3 ^{vi} —P1—O1	111.07 (8)
O1 ⁱⁱ —Ca1—P1 ^{iv}	93.00 (4)	O3—P1—O1	111.07 (8)
O1—Ca1—P1 ^{iv}	166.60 (5)	O3 ^{vi} —P1—O2	108.05 (8)
O2 ⁱⁱⁱ —Ca1—P1 ^{iv}	66.19 (5)	O3—P1—O2	108.05 (8)
O2 ^{iv} —Ca1—P1 ^{iv}	27.74 (5)	O1—P1—O2	111.08 (13)
O2 ^v —Ca1—P1 ^{iv}	98.63 (5)	O3 ^{vi} —P1—Ca2	53.91 (6)
O3 ^{iv} —Ca1—P1 ^{iv}	28.56 (3)	O3—P1—Ca2	53.91 (6)
O3 ⁱⁱⁱ —Ca1—P1 ^{iv}	122.12 (4)	O1—P1—Ca2	133.39 (9)
O3 ^v —Ca1—P1 ^{iv}	93.56 (4)	O2—P1—Ca2	115.53 (9)
P1 ⁱⁱⁱ —Ca1—P1 ^{iv}	93.667 (19)	O3 ^{vi} —P1—Ca1 ^{xii}	61.06 (7)
O1 ⁱ —Ca1—P1 ^v	166.60 (5)	O3—P1—Ca1 ^{xii}	112.64 (7)
O1 ⁱⁱ —Ca1—P1 ^v	97.50 (5)	O1—P1—Ca1 ^{xii}	135.78 (6)
O1—Ca1—P1 ^v	93.00 (4)	O2—P1—Ca1 ^{xii}	47.89 (6)
O2 ⁱⁱⁱ —Ca1—P1 ^v	98.63 (5)	Ca2—P1—Ca1 ^{xii}	80.163 (19)
O2 ^{iv} —Ca1—P1 ^v	66.19 (5)	O3 ^{vi} —P1—Ca1 ^v	112.64 (7)
O2 ^v —Ca1—P1 ^v	27.74 (5)	O3—P1—Ca1 ^v	61.06 (7)
O3 ^{iv} —Ca1—P1 ^v	122.12 (4)	O1—P1—Ca1 ^v	135.78 (6)
O3 ⁱⁱⁱ —Ca1—P1 ^v	93.56 (4)	O2—P1—Ca1 ^v	47.89 (6)
O3 ^v —Ca1—P1 ^v	28.56 (3)	Ca2—P1—Ca1 ^v	80.163 (19)
P1 ⁱⁱⁱ —Ca1—P1 ^v	93.667 (19)	Ca1 ^{xii} —P1—Ca1 ^v	65.25 (3)
P1 ^{iv} —Ca1—P1 ^v	93.667 (19)	O3 ^{vi} —P1—Ca2 ^{xiii}	79.55 (7)
O4—Ca2—O4 ^{vi}	6.9 (5)	O3—P1—Ca2 ^{xiii}	79.55 (7)
O4—Ca2—O3 ^{vii}	106.1 (2)	O1—P1—Ca2 ^{xiii}	55.21 (9)

O4 ^{vi} —Ca2—O3 ^{vii}	99.5 (2)	O2—P1—Ca2 ^{xiii}	166.28 (9)
O4—Ca2—O3 ^{viii}	99.5 (2)	Ca2—P1—Ca2 ^{xiii}	78.18 (3)
O4 ^{vi} —Ca2—O3 ^{vii}	106.1 (2)	Ca1 ^{xii} —P1—Ca2 ^{xiii}	140.554 (19)
O3 ^{vii} —Ca2—O3 ^{viii}	139.87 (9)	Ca1 ^v —P1—Ca2 ^{xiii}	140.554 (19)
O4—Ca2—O2 ^{ix}	152.29 (7)	O3 ^{vi} —P1—Ca2 ^{xiv}	122.57 (7)
O4 ^{vi} —Ca2—O2 ^{ix}	152.29 (7)	O3—P1—Ca2 ^{xiv}	122.57 (7)
O3 ^{vii} —Ca2—O2 ^{ix}	85.66 (4)	O1—P1—Ca2 ^{xiv}	77.28 (9)
O3 ^{viii} —Ca2—O2 ^{ix}	85.66 (4)	O2—P1—Ca2 ^{xiv}	33.79 (8)
O4—Ca2—O3	83.45 (13)	Ca2—P1—Ca2 ^{xiv}	149.32 (3)
O4 ^{vi} —Ca2—O3	80.03 (13)	Ca1 ^{xii} —P1—Ca2 ^{xiv}	74.110 (17)
O3 ^{vii} —Ca2—O3	77.97 (3)	Ca1 ^v —P1—Ca2 ^{xiv}	74.110 (17)
O3 ^{viii} —Ca2—O3	136.14 (6)	Ca2 ^{xiii} —P1—Ca2 ^{xiv}	132.49 (3)
O2 ^{ix} —Ca2—O3	74.43 (6)	P1—O1—Ca1 ^{vi}	129.76 (6)
O4—Ca2—O3 ^{vi}	80.03 (13)	P1—O1—Ca1	129.76 (6)
O4 ^{vi} —Ca2—O3 ^{vi}	83.45 (13)	Ca1 ^{vi} —O1—Ca1	91.19 (8)
O3 ^{vii} —Ca2—O3 ^{vi}	136.14 (6)	P1—O1—Ca2 ^{xiii}	96.89 (10)
O3 ^{viii} —Ca2—O3 ^{vi}	77.97 (3)	Ca1 ^{vi} —O1—Ca2 ^{xiii}	101.83 (7)
O2 ^{ix} —Ca2—O3 ^{vi}	74.44 (6)	Ca1—O1—Ca2 ^{xiii}	101.83 (7)
O3—Ca2—O3 ^{vi}	59.31 (8)	P1—O2—Ca2 ^{xiv}	125.03 (12)
O4—Ca2—O1 ^x	106.70 (5)	P1—O2—Ca1 ^v	104.37 (8)
O4 ^{vi} —Ca2—O1 ^x	106.70 (5)	Ca2 ^{xiv} —O2—Ca1 ^v	113.73 (7)
O3 ^{vii} —Ca2—O1 ^x	71.66 (4)	P1—O2—Ca1 ^{xii}	104.37 (8)
O3 ^{viii} —Ca2—O1 ^x	71.66 (4)	Ca2 ^{xiv} —O2—Ca1 ^{xii}	113.73 (7)
O2 ^{ix} —Ca2—O1 ^x	100.78 (7)	Ca1 ^v —O2—Ca1 ^{xii}	89.50 (8)
O3—Ca2—O1 ^x	149.56 (4)	P1—O3—Ca2 ⁱⁱⁱ	142.14 (9)
O3 ^{vi} —Ca2—O1 ^x	149.56 (4)	P1—O3—Ca2	96.34 (8)
O4—Ca2—P1	83.00 (2)	Ca2 ⁱⁱⁱ —O3—Ca2	117.45 (7)
O4 ^{vi} —Ca2—P1	83.00 (2)	P1—O3—Ca1 ^v	90.38 (8)
O3 ^{vii} —Ca2—P1	106.68 (4)	Ca2 ⁱⁱⁱ —O3—Ca1 ^v	99.88 (6)
O3 ^{viii} —Ca2—P1	106.68 (4)	Ca2—O3—Ca1 ^v	99.19 (5)
O2 ^{ix} —Ca2—P1	69.50 (6)	O4 ^{vi} —O4—Ca2 ^x	86.6 (2)
O3—Ca2—P1	29.75 (4)	O4 ^{vi} —O4—Ca2 ^{xiii}	86.6 (2)
O3 ^{vi} —Ca2—P1	29.75 (4)	Ca2 ^x —O4—Ca2 ^{xiii}	119.65 (5)
O1 ^x —Ca2—P1	170.28 (5)	O4 ^{vi} —O4—Ca2	86.6 (2)
O4—Ca2—P1 ^x	78.85 (2)	Ca2 ^x —O4—Ca2	119.65 (5)
O4 ^{vi} —Ca2—P1 ^x	78.85 (2)	Ca2 ^{xiii} —O4—Ca2	119.65 (5)
O3 ^{vii} —Ca2—P1 ^x	77.65 (4)	O4 ^{vi} —O4—H1	0.000 (5)
O3 ^{viii} —Ca2—P1 ^x	77.65 (4)	Ca2 ^x —O4—H1	86.6 (2)
O2 ^{ix} —Ca2—P1 ^x	128.68 (6)	Ca2 ^{xiii} —O4—H1	86.6 (2)
O3—Ca2—P1 ^x	144.39 (4)	Ca2—O4—H1	86.6 (2)
O3 ^{vi} —Ca2—P1 ^x	144.39 (4)	O4 ^{vi} —O4—H1 ^{vi}	180.000 (14)
O1 ^x —Ca2—P1 ^x	27.90 (5)	Ca2 ^x —O4—H1 ^{vi}	93.4 (2)
P1—Ca2—P1 ^x	161.82 (3)	Ca2 ^{xiii} —O4—H1 ^{vi}	93.4 (2)
O4—Ca2—P1 ^{ix}	172.80 (12)	Ca2—O4—H1 ^{vi}	93.4 (2)
O4 ^{vi} —Ca2—P1 ^{ix}	172.79 (12)	H1—O4—H1 ^{vi}	180.0

Symmetry codes: (i) $-y+1, x-y, z$; (ii) $-x+y+1, -x+1, z$; (iii) $y, -x+y, -z$; (iv) $x-y+1, x, -z$; (v) $-x+1, -y+1, -z$; (vi) $x, y, -z+1/2$; (vii) $x-y, x, -z$; (viii) $x-y, x, z+1/2$; (ix) $-x+y, -x+1, z$; (x) $-y, x-y, z$; (xi) $x-1, y, z$; (xii) $-x+1, -y+1, z+1/2$; (xiii) $-x+y, -x, z$; (xiv) $-y+1, x-y+1, z$.