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Bis(nitrato-κ^2O,O')(1,4,7,10,13-pentaoxacyclopentadecane)calcium(II)

Michael D. Brown, William Levason and Michael Webster*

School of Chemistry, University of Southampton, Southampton SO17 1BJ, England

Correspondence e-mail: m.webster@soton.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.089
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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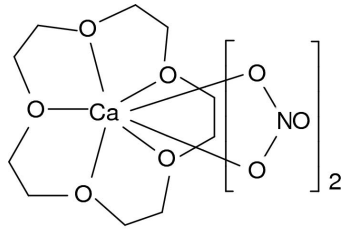
The crystal structure of the title compound, $[Ca(NO_3)_2(C_{10}H_{20}O_5)]$, at 120 K contains discrete molecules with nine-coordinate Ca atoms. There are two molecules in the asymmetric unit, related by a pseudo-inversion centre. The crown bonds through five O atoms [Ca—O = 2.464 (2)–2.567 (2) Å] and the nitrates are bidentate [Ca—O = 2.444 (2)–2.588 (2) Å]. The structure is a polymorph of a previously reported room-temperature form.

Comment

A room-temperature crystal structure of the title compound, (I), has been reported in the space group *Pbca* (No. 61) (Junk & Steed, 1999). There appears to be a typographical error in the cell dimensions reported in the paper (*a* and *c* have been interchanged) when compared with the values in the deposited CIF.



(I)

Our orthorhombic cell parameters were similar to the published values with, as expected, slightly smaller values due to the lower temperature (cell volume *ca* 2.7% smaller). However, the observed absences were not consistent with space group *Pbca*, but rather with space group $Pca2_1$ (No. 29) or *Pbcm* (No. 57) (both referred to standard settings). No solution emerged in the centrosymmetric space group *Pbcm*, but a solution did result from a direct methods calculation in $Pca2_1$, with two similar molecules in the asymmetric unit. The Flack (1983) parameter indicates an inversion twin.

There is a pseudo-centre of symmetry relating the two molecules and the solution in the space group *Pbca* was explored, even though well over half of the reflections were 'observed' in the *h*0*l* zone with *l* odd (in the appropriate orientation). Although a solution with one molecule in the asymmetric unit could be obtained, refinement failed to reduce $R1$ below 0.18 and the displacement ellipsoids were very elongated.

The conclusion is that, at 120 K, the crystal structure is correctly described in the non-centrosymmetric space group $Pca2_1$ and represents a polymorph of the room-temperature structure.

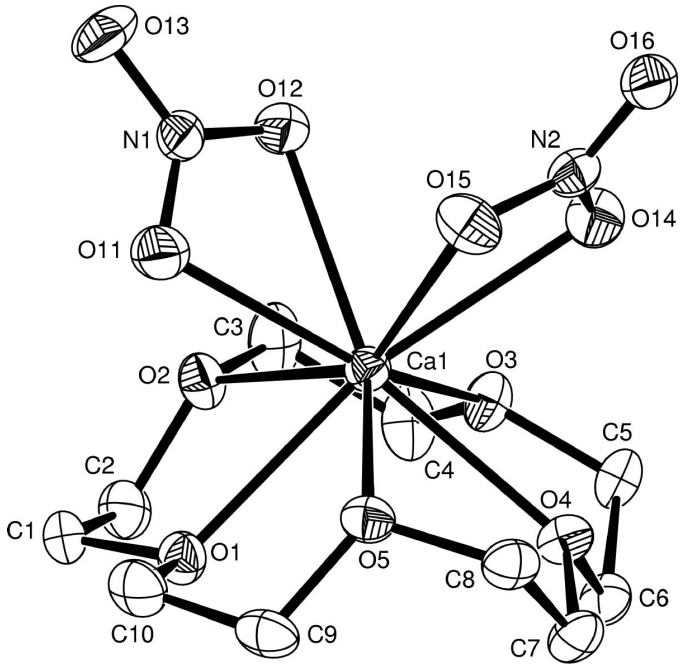


Figure 1
One of the two molecules in the asymmetric unit of $[Ca(NO_3)_2(15\text{-crown-}5)]$, showing the atom-labelling scheme. Ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity. The other molecule is very similar.

On transforming the data to the *Pbca* orientation, the systematic absences correspond to the non-standard space group setting $Pb2_1a$ (No. 29), which is a maximal non-isomorphic subgroup of *Pbca*. Whether this polymorph is stable at room temperature or a structural change occurs on cooling is not clear; however, the relationship between the two structures perhaps favours the latter.

The geometry agrees well with the earlier room-temperature structure (Junk & Steed, 1999). The Ca atoms are nine-coordinate with two bidentate nitrate groups (Fig. 1 and Table 1). The Ca—O bonds to the crown ligands [2.464 (2)–2.567 (2) Å] can be compared with the literature values [2.474 (3)–2.581 (4) Å; Junk & Steed, 1999]. The nitrates are bonded fairly symmetrically [differences in Ca—O within each ligand range from 0.006 (3) to 0.144 (3) Å] and, as noted before (Valle *et al.*, 1986), the terminal N—O bond is shorter than the bridging bonds by *ca* 0.04 Å; values for one typical ligand are included in Table 1. There is also a distortion of the angles at nitrogen, the O—N—O angle involved in the four-membered ring being several degrees smaller than the ideal value of 120°.

Experimental

Crystals were isolated during the attempted crystal growth of a calcium azide/15-crown-5 complex. The nitrate was present in the mixture in small amounts from the synthesis $[Ca(NO_3)_2(15\text{-crown-}5)$ and CsN_3 in methanol] and led to the isolated product.

Crystal data

$[Ca(NO_3)_2(C_{10}H_{20}O_5)]$
$M_r = 384.36$
Orthorhombic, $Pca2_1$
$a = 15.1940\ (15)$ Å
$b = 15.908\ (3)$ Å
$c = 13.227\ (2)$ Å
$V = 3197.1\ (8)$ Å^3
$Z = 8$
$D_x = 1.597$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3946 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.45$ mm^{-1}
$T = 120\ (2)$ K
Plate, colourless
$0.22 \times 0.17 \times 0.03$ mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.814$, $T_{max} = 0.986$
24234 measured reflections
6509 independent reflections
5672 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 27.5°$
$h = -18 \rightarrow 19$
$k = -20 \rightarrow 18$
$l = -17 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.089$
$S = 1.03$
6509 reflections
435 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 0.774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Absolute structure: Flack (1983), 2675 Friedel pairs
Flack parameter = 0.48 (3)

Table 1
Selected geometric parameters (Å, °).

Ca1—O1	2.514 (2)	Ca2—O8	2.464 (2)
Ca1—O2	2.561 (2)	Ca2—O9	2.502 (2)
Ca1—O3	2.4759 (19)	Ca2—O10	2.514 (2)
Ca1—O4	2.476 (2)	Ca2—O17	2.453 (2)
Ca1—O5	2.523 (2)	Ca2—O18	2.502 (2)
Ca1—O11	2.454 (2)	Ca2—O20	2.448 (2)
Ca1—O12	2.460 (2)	Ca2—O21	2.548 (2)
Ca1—O14	2.588 (2)	N1—O11	1.268 (3)
Ca1—O15	2.444 (2)	N1—O12	1.263 (3)
Ca2—O6	2.539 (2)	N1—O13	1.226 (3)
Ca2—O7	2.567 (2)		
O4—Ca1—O3	66.82 (6)	O10—Ca2—O6	64.58 (7)
O4—Ca1—O5	66.15 (6)	O8—Ca2—O7	64.85 (7)
O1—Ca1—O5	64.39 (7)	O6—Ca2—O7	64.10 (7)
O3—Ca1—O2	65.25 (6)	O17—Ca2—O18	51.94 (7)
O1—Ca1—O2	64.45 (7)	O20—Ca2—O21	50.99 (7)
O11—Ca1—O12	52.36 (7)	O13—N1—O12	121.1 (3)
O15—Ca1—O14	50.61 (7)	O13—N1—O11	121.1 (3)
O8—Ca2—O9	66.28 (6)	O12—N1—O11	117.8 (2)
O9—Ca2—O10	65.58 (6)		

H atoms were placed in calculated positions (C—H = 0.99 Å) with a common refined U_{iso}.

Data collection: *COLLECT* (Hooft, 1998) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *COLLECT* and *DENZO*; data reduction: *COLLECT* and *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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supporting information

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$h = -18\rightarrow19$
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Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.089$
$S = 1.03$
6509 reflections
435 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0324P)^2 + 0.774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Absolute structure: Flack (1983), 2675 Friedel pairs
Absolute structure parameter: 0.48 (3)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.
H atoms were placed in calculated positions with a common refined isotropic adp. Two *SHELXL* DELU commands were used to constrain N2—O16 and N3—O18 adp components.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ca1	0.05736 (3)	0.57918 (4)	0.63467 (4)	0.01992 (13)
Ca2	0.07350 (3)	0.06744 (4)	0.68675 (4)	0.02071 (13)
O1	0.06629 (12)	0.66896 (13)	0.79072 (16)	0.0244 (5)
O2	−0.03808 (12)	0.71183 (12)	0.63316 (17)	0.0264 (4)
O3	−0.10165 (12)	0.55365 (12)	0.60764 (16)	0.0246 (5)
O4	0.00142 (11)	0.45523 (14)	0.72796 (15)	0.0239 (5)
O5	0.16019 (12)	0.52707 (13)	0.77065 (15)	0.0246 (4)
O6	0.08852 (12)	0.15369 (13)	0.52612 (16)	0.0258 (5)
O7	−0.00591 (12)	0.20987 (13)	0.68624 (17)	0.0297 (5)
O8	−0.08743 (12)	0.06023 (13)	0.70818 (18)	0.0286 (5)
O9	0.00423 (11)	−0.05636 (13)	0.60148 (15)	0.0229 (4)
O10	0.16604 (12)	0.00232 (13)	0.55007 (16)	0.0248 (4)
C1	0.0368 (2)	0.75372 (19)	0.7780 (2)	0.0297 (7)
H1A	0.0781	0.7853	0.7343	0.0332 (13)*
H1B	0.0332	0.7824	0.8443	0.0332 (13)*
C2	−0.0519 (2)	0.7492 (2)	0.7301 (2)	0.0308 (7)
H2A	−0.0922	0.7143	0.7714	0.0332 (13)*
H2B	−0.0775	0.8061	0.7230	0.0332 (13)*
C3	−0.1181 (2)	0.6982 (2)	0.5775 (3)	0.0355 (8)
H3A	−0.1044	0.6922	0.5047	0.0332 (13)*
H3B	−0.1574	0.7474	0.5857	0.0332 (13)*
C4	−0.16399 (18)	0.6209 (2)	0.6141 (3)	0.0322 (8)
H4A	−0.1839	0.6284	0.6848	0.0332 (13)*
H4B	−0.2160	0.6087	0.5714	0.0332 (13)*
C5	−0.13424 (17)	0.47439 (18)	0.6444 (3)	0.0253 (6)
H5A	−0.1206	0.4295	0.5950	0.0332 (13)*
H5B	−0.1990	0.4773	0.6524	0.0332 (13)*
C6	−0.09226 (17)	0.4543 (2)	0.7442 (2)	0.0248 (7)
H6A	−0.1090	0.4968	0.7954	0.0332 (13)*
H6B	−0.1115	0.3983	0.7682	0.0332 (13)*
C7	0.05164 (19)	0.4206 (2)	0.8107 (2)	0.0270 (7)
H7A	0.0415	0.3593	0.8162	0.0332 (13)*
H7B	0.0344	0.4474	0.8753	0.0332 (13)*
C8	0.14598 (19)	0.4382 (2)	0.7877 (2)	0.0267 (7)
H8A	0.1830	0.4191	0.8449	0.0332 (13)*
H8B	0.1638	0.4063	0.7268	0.0332 (13)*
C9	0.16558 (19)	0.5742 (2)	0.8640 (2)	0.0296 (7)
H9A	0.2242	0.5667	0.8954	0.0332 (13)*

H9B	0.1202	0.5546	0.9122	0.0332 (13)*
C10	0.15087 (19)	0.6645 (2)	0.8381 (2)	0.0313 (7)
H10A	0.1520	0.6995	0.9000	0.0332 (13)*
H10B	0.1972	0.6847	0.7915	0.0332 (13)*
C11	0.0744 (2)	0.2423 (2)	0.5396 (3)	0.0326 (7)
H11A	0.0740	0.2712	0.4733	0.0332 (13)*
H11B	0.1219	0.2668	0.5815	0.0332 (13)*
C12	−0.0122 (2)	0.2524 (2)	0.5906 (3)	0.0339 (7)
H12A	−0.0254	0.3127	0.6010	0.0332 (13)*
H12B	−0.0596	0.2274	0.5490	0.0332 (13)*
C13	−0.0875 (2)	0.2044 (2)	0.7390 (3)	0.0401 (9)
H13A	−0.1204	0.2577	0.7303	0.0332 (13)*
H13B	−0.0759	0.1968	0.8120	0.0332 (13)*
C14	−0.14260 (19)	0.1328 (2)	0.7013 (3)	0.0353 (8)
H14A	−0.1958	0.1258	0.7437	0.0332 (13)*
H14B	−0.1611	0.1426	0.6305	0.0332 (13)*
C15	−0.12943 (17)	−0.01721 (18)	0.6792 (3)	0.0264 (6)
H15A	−0.1931	−0.0075	0.6684	0.0332 (13)*
H15B	−0.1226	−0.0593	0.7337	0.0332 (13)*
C16	−0.08866 (18)	−0.0496 (2)	0.5839 (2)	0.0248 (6)
H16A	−0.1135	−0.1052	0.5665	0.0332 (13)*
H16B	−0.1004	−0.0105	0.5273	0.0332 (13)*
C17	0.04986 (19)	−0.0988 (2)	0.5207 (2)	0.0275 (7)
H17A	0.0327	−0.0748	0.4545	0.0332 (13)*
H17B	0.0355	−0.1595	0.5209	0.0332 (13)*
C18	0.14651 (19)	−0.0858 (2)	0.5393 (2)	0.0278 (7)
H18A	0.1642	−0.1160	0.6016	0.0332 (13)*
H18B	0.1806	−0.1093	0.4821	0.0332 (13)*
C19	0.1708 (2)	0.0438 (2)	0.4544 (2)	0.0307 (7)
H19A	0.1203	0.0272	0.4115	0.0332 (13)*
H19B	0.2259	0.0281	0.4191	0.0332 (13)*
C20	0.16898 (19)	0.1361 (2)	0.4732 (2)	0.0311 (7)
H20A	0.2203	0.1532	0.5145	0.0332 (13)*
H20B	0.1708	0.1672	0.4084	0.0332 (13)*
N1	0.15064 (15)	0.69136 (16)	0.50441 (19)	0.0256 (6)
N2	0.12184 (16)	0.45287 (16)	0.49052 (19)	0.0245 (5)
N3	0.17255 (16)	0.19009 (16)	0.7974 (2)	0.0286 (6)
N4	0.12030 (15)	−0.05703 (16)	0.83964 (19)	0.0236 (5)
O11	0.17180 (14)	0.68333 (15)	0.59664 (17)	0.0336 (5)
O12	0.08380 (13)	0.65180 (14)	0.47334 (16)	0.0291 (5)
O13	0.19341 (14)	0.73635 (15)	0.44738 (18)	0.0380 (6)
O14	0.03969 (13)	0.46190 (14)	0.50064 (18)	0.0309 (5)
O15	0.17028 (13)	0.49595 (15)	0.54919 (18)	0.0338 (5)
O16	0.15427 (14)	0.40636 (14)	0.42598 (17)	0.0318 (5)
O17	0.19799 (13)	0.16340 (14)	0.71155 (16)	0.0309 (5)
O18	0.11277 (14)	0.14898 (14)	0.84208 (17)	0.0317 (5)
O19	0.20596 (14)	0.25334 (14)	0.83513 (18)	0.0390 (6)
O20	0.17272 (13)	−0.03119 (15)	0.77149 (16)	0.0297 (5)

O21	0.04135 (13)	−0.03286 (14)	0.83236 (17)	0.0277 (5)
O22	0.14603 (14)	−0.10248 (15)	0.90865 (17)	0.0327 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0196 (2)	0.0212 (3)	0.0190 (3)	−0.0011 (2)	−0.0005 (2)	0.0005 (2)
Ca2	0.0211 (3)	0.0220 (3)	0.0190 (3)	−0.0021 (2)	0.0007 (2)	−0.0015 (3)
O1	0.0248 (10)	0.0232 (12)	0.0253 (11)	−0.0018 (8)	−0.0037 (8)	−0.0003 (9)
O2	0.0281 (10)	0.0234 (11)	0.0277 (11)	−0.0023 (8)	−0.0035 (9)	−0.0042 (10)
O3	0.0194 (9)	0.0187 (10)	0.0357 (13)	0.0038 (8)	0.0001 (8)	0.0039 (9)
O4	0.0182 (10)	0.0299 (12)	0.0236 (11)	−0.0006 (8)	−0.0009 (8)	0.0042 (9)
O5	0.0253 (10)	0.0283 (12)	0.0201 (11)	0.0004 (9)	−0.0015 (8)	0.0003 (9)
O6	0.0280 (10)	0.0235 (11)	0.0260 (11)	−0.0048 (8)	0.0052 (9)	0.0038 (9)
O7	0.0359 (11)	0.0209 (10)	0.0323 (11)	−0.0011 (8)	0.0050 (10)	0.0031 (10)
O8	0.0213 (10)	0.0183 (11)	0.0463 (15)	0.0025 (8)	−0.0036 (9)	−0.0054 (10)
O9	0.0196 (10)	0.0289 (12)	0.0202 (11)	−0.0003 (8)	0.0007 (7)	−0.0049 (8)
O10	0.0246 (10)	0.0286 (12)	0.0211 (11)	−0.0008 (8)	0.0010 (8)	−0.0004 (9)
C1	0.0438 (18)	0.0194 (17)	0.0260 (16)	−0.0060 (13)	0.0026 (13)	−0.0038 (13)
C2	0.0380 (16)	0.0220 (17)	0.0324 (17)	0.0051 (14)	0.0009 (13)	−0.0015 (14)
C3	0.0339 (17)	0.0226 (17)	0.050 (2)	0.0046 (13)	−0.0173 (15)	0.0024 (15)
C4	0.0192 (13)	0.0258 (17)	0.052 (2)	0.0060 (11)	−0.0049 (13)	−0.0050 (15)
C5	0.0207 (13)	0.0198 (15)	0.0355 (17)	−0.0019 (11)	−0.0005 (13)	0.0051 (14)
C6	0.0179 (13)	0.0263 (17)	0.0302 (17)	−0.0023 (11)	0.0070 (12)	−0.0005 (13)
C7	0.0294 (16)	0.0264 (17)	0.0254 (17)	−0.0001 (12)	−0.0037 (12)	0.0090 (13)
C8	0.0285 (16)	0.0277 (18)	0.0237 (16)	0.0053 (12)	−0.0007 (12)	0.0043 (13)
C9	0.0270 (15)	0.043 (2)	0.0189 (15)	−0.0020 (13)	−0.0039 (12)	−0.0025 (14)
C10	0.0266 (15)	0.040 (2)	0.0273 (17)	−0.0067 (13)	−0.0065 (12)	−0.0044 (14)
C11	0.0465 (18)	0.0229 (17)	0.0283 (17)	−0.0073 (14)	0.0010 (14)	0.0054 (13)
C12	0.0431 (18)	0.0237 (18)	0.0349 (18)	0.0038 (14)	−0.0035 (14)	0.0050 (14)
C13	0.0427 (19)	0.0243 (18)	0.053 (2)	0.0030 (14)	0.0160 (16)	−0.0033 (16)
C14	0.0256 (15)	0.0272 (18)	0.053 (2)	0.0078 (12)	0.0064 (14)	0.0039 (16)
C15	0.0194 (13)	0.0208 (15)	0.0389 (18)	−0.0034 (11)	0.0002 (13)	−0.0004 (14)
C16	0.0205 (14)	0.0280 (17)	0.0260 (16)	−0.0049 (12)	−0.0036 (12)	0.0005 (13)
C17	0.0302 (15)	0.0279 (17)	0.0242 (16)	−0.0008 (13)	0.0043 (12)	−0.0074 (13)
C18	0.0295 (15)	0.0299 (18)	0.0241 (16)	0.0028 (13)	0.0026 (12)	−0.0049 (14)
C19	0.0240 (14)	0.046 (2)	0.0217 (16)	−0.0013 (13)	0.0056 (12)	−0.0005 (14)
C20	0.0270 (15)	0.041 (2)	0.0254 (16)	−0.0085 (13)	0.0059 (12)	0.0060 (14)
N1	0.0291 (13)	0.0195 (14)	0.0281 (14)	0.0015 (10)	0.0089 (11)	−0.0028 (11)
N2	0.0268 (13)	0.0229 (14)	0.0237 (14)	0.0013 (10)	0.0002 (10)	0.0060 (9)
N3	0.0311 (13)	0.0240 (15)	0.0306 (15)	0.0031 (11)	−0.0116 (11)	0.0004 (11)
N4	0.0230 (12)	0.0264 (14)	0.0213 (13)	−0.0023 (10)	−0.0019 (10)	−0.0060 (11)
O11	0.0340 (11)	0.0390 (14)	0.0276 (12)	−0.0093 (10)	0.0007 (9)	−0.0018 (10)
O12	0.0336 (11)	0.0302 (12)	0.0237 (11)	−0.0035 (9)	−0.0014 (9)	0.0012 (9)
O13	0.0384 (12)	0.0325 (13)	0.0430 (14)	0.0014 (10)	0.0198 (10)	0.0127 (11)
O14	0.0259 (11)	0.0315 (13)	0.0352 (13)	0.0016 (9)	0.0025 (9)	0.0000 (10)
O15	0.0282 (11)	0.0428 (15)	0.0305 (13)	0.0034 (10)	−0.0058 (9)	−0.0058 (11)
O16	0.0381 (12)	0.0259 (12)	0.0314 (12)	0.0036 (9)	0.0071 (9)	0.0015 (9)

O17	0.0323 (11)	0.0341 (12)	0.0264 (12)	−0.0081 (9)	−0.0011 (8)	−0.0004 (9)
O18	0.0378 (12)	0.0311 (13)	0.0263 (11)	−0.0053 (10)	−0.0001 (9)	−0.0001 (10)
O19	0.0418 (12)	0.0237 (12)	0.0516 (15)	0.0003 (10)	−0.0188 (11)	−0.0093 (11)
O20	0.0270 (11)	0.0362 (13)	0.0257 (12)	0.0021 (9)	0.0016 (9)	0.0002 (10)
O21	0.0223 (10)	0.0319 (13)	0.0290 (12)	0.0002 (9)	−0.0007 (8)	0.0023 (10)
O22	0.0360 (12)	0.0310 (13)	0.0312 (13)	0.0009 (10)	−0.0095 (9)	0.0020 (10)

Geometric parameters (Å, º)

Ca1—O1	2.514 (2)	C5—C6	1.501 (4)
Ca1—O2	2.561 (2)	C5—H5A	0.990
Ca1—O3	2.4759 (19)	C5—H5B	0.990
Ca1—O4	2.476 (2)	C6—H6A	0.990
Ca1—O5	2.523 (2)	C6—H6B	0.990
Ca1—O11	2.454 (2)	C7—C8	1.492 (4)
Ca1—O12	2.460 (2)	C7—H7A	0.990
Ca1—O14	2.588 (2)	C7—H7B	0.990
Ca1—O15	2.444 (2)	C8—H8A	0.990
Ca1—N1	2.857 (3)	C8—H8B	0.990
Ca1—N2	2.938 (3)	C9—C10	1.493 (5)
Ca2—O6	2.539 (2)	C9—H9A	0.990
Ca2—O7	2.567 (2)	C9—H9B	0.990
Ca2—O8	2.464 (2)	C10—H10A	0.990
Ca2—O9	2.502 (2)	C10—H10B	0.990
Ca2—O10	2.514 (2)	C11—C12	1.487 (4)
Ca2—O17	2.453 (2)	C11—H11A	0.990
Ca2—O18	2.502 (2)	C11—H11B	0.990
Ca2—O20	2.448 (2)	C12—H12A	0.990
Ca2—O21	2.548 (2)	C12—H12B	0.990
Ca2—N3	2.866 (3)	C13—C14	1.499 (5)
Ca2—N4	2.918 (3)	C13—H13A	0.990
O1—C1	1.430 (4)	C13—H13B	0.990
O1—C10	1.432 (3)	C14—H14A	0.990
O2—C2	1.429 (4)	C14—H14B	0.990
O2—C3	1.438 (3)	C15—C16	1.495 (4)
O3—C4	1.431 (3)	C15—H15A	0.990
O3—C5	1.439 (3)	C15—H15B	0.990
O4—C6	1.439 (3)	C16—H16A	0.990
O4—C7	1.444 (3)	C16—H16B	0.990
O5—C9	1.447 (4)	C17—C18	1.503 (4)
O5—C8	1.449 (4)	C17—H17A	0.990
O6—C20	1.436 (3)	C17—H17B	0.990
O6—C11	1.437 (4)	C18—H18A	0.990
O7—C13	1.425 (4)	C18—H18B	0.990
O7—C12	1.437 (4)	C19—C20	1.489 (5)
O8—C14	1.429 (3)	C19—H19A	0.990
O8—C15	1.439 (3)	C19—H19B	0.990
O9—C16	1.434 (3)	C20—H20A	0.990

O9—C17	1.441 (3)	C20—H20B	0.990
O10—C19	1.429 (4)	N1—O11	1.268 (3)
O10—C18	1.440 (4)	N1—O12	1.263 (3)
C1—C2	1.491 (4)	N1—O13	1.226 (3)
C1—H1A	0.990	N2—O16	1.232 (3)
C1—H1B	0.990	N2—O14	1.264 (3)
C2—H2A	0.990	N2—O15	1.270 (3)
C2—H2B	0.990	N3—O19	1.233 (3)
C3—C4	1.495 (5)	N3—O18	1.266 (3)
C3—H3A	0.990	N3—O17	1.272 (3)
C3—H3B	0.990	N4—O22	1.228 (3)
C4—H4A	0.990	N4—O21	1.263 (3)
C4—H4B	0.990	N4—O20	1.271 (3)

O15—Ca1—O11	76.91 (8)	O2—C2—C1	105.6 (2)
O15—Ca1—O12	74.84 (8)	O2—C2—H2A	110.6
O15—Ca1—O4	92.30 (8)	C1—C2—H2A	110.6
O11—Ca1—O4	152.00 (7)	O2—C2—H2B	110.6
O12—Ca1—O4	149.58 (7)	C1—C2—H2B	110.6
O15—Ca1—O3	121.96 (7)	H2A—C2—H2B	108.8
O11—Ca1—O3	140.59 (7)	O2—C3—C4	110.6 (2)
O12—Ca1—O3	96.38 (7)	O2—C3—H3A	109.5
O4—Ca1—O3	66.82 (6)	C4—C3—H3A	109.5
O15—Ca1—O1	130.52 (7)	O2—C3—H3B	109.5
O11—Ca1—O1	75.31 (7)	C4—C3—H3B	109.5
O12—Ca1—O1	115.89 (7)	H3A—C3—H3B	108.1
O4—Ca1—O1	93.55 (7)	O3—C4—C3	106.7 (2)
O3—Ca1—O1	105.34 (7)	O3—C4—H4A	110.4
O15—Ca1—O5	73.56 (7)	C3—C4—H4A	110.4
O11—Ca1—O5	85.94 (7)	O3—C4—H4B	110.4
O12—Ca1—O5	132.20 (7)	C3—C4—H4B	110.4
O4—Ca1—O5	66.15 (6)	H4A—C4—H4B	108.6
O3—Ca1—O5	130.81 (7)	O3—C5—C6	109.7 (2)
O1—Ca1—O5	64.39 (7)	O3—C5—H5A	109.7
O15—Ca1—O2	147.17 (8)	C6—C5—H5A	109.7
O11—Ca1—O2	80.98 (7)	O3—C5—H5B	109.7
O12—Ca1—O2	72.46 (7)	C6—C5—H5B	109.7
O4—Ca1—O2	117.76 (7)	H5A—C5—H5B	108.2
O3—Ca1—O2	65.25 (6)	O4—C6—C5	106.7 (2)
O1—Ca1—O2	64.45 (7)	O4—C6—H6A	110.4
O5—Ca1—O2	128.84 (7)	C5—C6—H6A	110.4
O11—Ca1—O12	52.36 (7)	O4—C6—H6B	110.4
O15—Ca1—O14	50.61 (7)	C5—C6—H6B	110.4
O11—Ca1—O14	114.82 (8)	H6A—C6—H6B	108.6
O12—Ca1—O14	76.18 (7)	O4—C7—C8	106.4 (2)
O4—Ca1—O14	74.44 (7)	O4—C7—H7A	110.5
O3—Ca1—O14	71.43 (7)	C8—C7—H7A	110.5
O1—Ca1—O14	167.92 (7)	O4—C7—H7B	110.5

O5—Ca1—O14	108.41 (7)	C8—C7—H7B	110.5
O2—Ca1—O14	122.01 (7)	H7A—C7—H7B	108.6
O15—Ca1—N1	73.21 (8)	O5—C8—C7	111.0 (2)
O11—Ca1—N1	26.24 (7)	O5—C8—H8A	109.4
O12—Ca1—N1	26.15 (7)	C7—C8—H8A	109.4
O4—Ca1—N1	165.49 (7)	O5—C8—H8B	109.4
O3—Ca1—N1	119.97 (7)	C7—C8—H8B	109.4
O1—Ca1—N1	96.51 (7)	H8A—C8—H8B	108.0
O5—Ca1—N1	109.14 (7)	O5—C9—C10	107.1 (2)
O2—Ca1—N1	76.20 (7)	O5—C9—H9A	110.3
O14—Ca1—N1	95.09 (7)	C10—C9—H9A	110.3
O15—Ca1—N2	25.22 (7)	O5—C9—H9B	110.3
O11—Ca1—N2	95.30 (7)	C10—C9—H9B	110.3
O12—Ca1—N2	72.77 (7)	H9A—C9—H9B	108.5
O4—Ca1—N2	83.87 (7)	O1—C10—C9	106.4 (2)
O3—Ca1—N2	96.87 (7)	O1—C10—H10A	110.4
O1—Ca1—N2	154.61 (7)	C9—C10—H10A	110.4
O5—Ca1—N2	91.80 (7)	O1—C10—H10B	110.4
O2—Ca1—N2	138.36 (7)	C9—C10—H10B	110.4
O14—Ca1—N2	25.44 (6)	H10A—C10—H10B	108.6
N1—Ca1—N2	82.55 (7)	O6—C11—C12	107.1 (2)
O20—Ca2—O17	82.11 (8)	O6—C11—H11A	110.3
O20—Ca2—O8	121.91 (7)	C12—C11—H11A	110.3
O17—Ca2—O8	141.15 (8)	O6—C11—H11B	110.3
O20—Ca2—O18	79.01 (8)	C12—C11—H11B	110.3
O8—Ca2—O18	99.57 (7)	H11A—C11—H11B	108.5
O20—Ca2—O9	87.76 (7)	O7—C12—C11	106.9 (2)
O17—Ca2—O9	151.01 (7)	O7—C12—H12A	110.3
O8—Ca2—O9	66.28 (6)	C11—C12—H12A	110.3
O18—Ca2—O9	151.49 (7)	O7—C12—H12B	110.3
O20—Ca2—O10	73.78 (7)	C11—C12—H12B	110.3
O17—Ca2—O10	85.49 (7)	H12A—C12—H12B	108.6
O8—Ca2—O10	128.21 (7)	O7—C13—C14	111.7 (3)
O18—Ca2—O10	132.13 (7)	O7—C13—H13A	109.3
O9—Ca2—O10	65.58 (6)	C14—C13—H13A	109.3
O20—Ca2—O6	132.39 (7)	O7—C13—H13B	109.3
O17—Ca2—O6	72.92 (7)	C14—C13—H13B	109.3
O8—Ca2—O6	102.15 (7)	H13A—C13—H13B	107.9
O18—Ca2—O6	112.67 (7)	O8—C14—C13	105.4 (2)
O9—Ca2—O6	94.93 (7)	O8—C14—H14A	110.7
O10—Ca2—O6	64.58 (7)	C13—C14—H14A	110.7
O17—Ca2—O21	115.88 (7)	O8—C14—H14B	110.7
O8—Ca2—O21	72.16 (7)	C13—C14—H14B	110.7
O18—Ca2—O21	75.51 (7)	H14A—C14—H14B	108.8
O9—Ca2—O21	76.54 (7)	O8—C15—C16	109.6 (2)
O10—Ca2—O21	113.13 (7)	O8—C15—H15A	109.7
O6—Ca2—O21	171.06 (7)	C16—C15—H15A	109.7
O20—Ca2—O7	148.93 (8)	O8—C15—H15B	109.7

O17—Ca2—O7	79.25 (7)	C16—C15—H15B	109.7
O8—Ca2—O7	64.85 (7)	H15A—C15—H15B	108.2
O18—Ca2—O7	69.92 (7)	O9—C16—C15	107.3 (2)
O9—Ca2—O7	119.73 (7)	O9—C16—H16A	110.3
O10—Ca2—O7	128.67 (7)	C15—C16—H16A	110.3
O6—Ca2—O7	64.10 (7)	O9—C16—H16B	110.3
O17—Ca2—O18	51.94 (7)	C15—C16—H16B	110.3
O20—Ca2—O21	50.99 (7)	H16A—C16—H16B	108.5
O21—Ca2—O7	117.68 (7)	O9—C17—C18	106.5 (2)
O20—Ca2—N3	83.06 (8)	O9—C17—H17A	110.4
O17—Ca2—N3	26.23 (7)	C18—C17—H17A	110.4
O8—Ca2—N3	119.61 (8)	O9—C17—H17B	110.4
O18—Ca2—N3	26.17 (7)	C18—C17—H17B	110.4
O9—Ca2—N3	170.79 (7)	H17A—C17—H17B	108.6
O10—Ca2—N3	110.74 (7)	O10—C18—C17	110.6 (2)
O6—Ca2—N3	90.69 (7)	O10—C18—H18A	109.5
O21—Ca2—N3	98.11 (8)	C17—C18—H18A	109.5
O7—Ca2—N3	69.34 (7)	O10—C18—H18B	109.5
O20—Ca2—N4	25.53 (7)	C17—C18—H18B	109.5
O17—Ca2—N4	98.15 (7)	H18A—C18—H18B	108.1
O8—Ca2—N4	97.50 (7)	O10—C19—C20	107.9 (2)
O18—Ca2—N4	74.02 (7)	O10—C19—H19A	110.1
O9—Ca2—N4	83.15 (7)	C20—C19—H19A	110.1
O10—Ca2—N4	94.73 (7)	O10—C19—H19B	110.1
O6—Ca2—N4	157.59 (7)	C20—C19—H19B	110.1
O21—Ca2—N4	25.59 (6)	H19A—C19—H19B	108.4
O7—Ca2—N4	135.66 (8)	O6—C20—C19	106.8 (2)
N3—Ca2—N4	88.87 (7)	O6—C20—H20A	110.4
C1—O1—C10	112.3 (2)	C19—C20—H20A	110.4
C1—O1—Ca1	114.99 (17)	O6—C20—H20B	110.4
C10—O1—Ca1	112.31 (17)	C19—C20—H20B	110.4
C2—O2—C3	113.5 (2)	H20A—C20—H20B	108.6
C2—O2—Ca1	114.75 (17)	O13—N1—O12	121.1 (3)
C3—O2—Ca1	111.03 (16)	O13—N1—O11	121.1 (3)
C4—O3—C5	114.0 (2)	O12—N1—O11	117.8 (2)
C4—O3—Ca1	120.98 (17)	O13—N1—Ca1	176.88 (19)
C5—O3—Ca1	115.52 (15)	O12—N1—Ca1	59.09 (14)
C6—O4—C7	114.0 (2)	O11—N1—Ca1	58.84 (14)
C6—O4—Ca1	114.94 (17)	O16—N2—O14	122.4 (3)
C7—O4—Ca1	120.02 (16)	O16—N2—O15	121.0 (2)
C9—O5—C8	112.4 (2)	O14—N2—O15	116.5 (3)
C9—O5—Ca1	118.23 (16)	O16—N2—Ca1	173.4 (2)
C8—O5—Ca1	109.86 (16)	O14—N2—Ca1	61.58 (15)
C20—O6—C11	112.3 (2)	O15—N2—Ca1	55.09 (14)
C20—O6—Ca2	112.27 (17)	O19—N3—O18	121.9 (3)
C11—O6—Ca2	114.39 (18)	O19—N3—O17	120.6 (3)
C13—O7—C12	113.7 (3)	O18—N3—O17	117.6 (2)
C13—O7—Ca2	110.72 (18)	O19—N3—Ca2	168.2 (2)

C12—O7—Ca2	116.67 (18)	O18—N3—Ca2	60.66 (14)
C14—O8—C15	114.5 (2)	O17—N3—Ca2	58.45 (13)
C14—O8—Ca2	122.48 (17)	O22—N4—O21	122.5 (2)
C15—O8—Ca2	116.68 (15)	O22—N4—O20	121.2 (2)
C16—O9—C17	112.9 (2)	O21—N4—O20	116.3 (2)
C16—O9—Ca2	115.32 (16)	O22—N4—Ca2	172.71 (19)
C17—O9—Ca2	120.03 (16)	O21—N4—Ca2	60.62 (14)
C19—O10—C18	111.9 (2)	O20—N4—Ca2	56.07 (14)
C19—O10—Ca2	118.35 (17)	N1—O11—Ca1	94.91 (16)
C18—O10—Ca2	110.91 (16)	N1—O12—Ca1	94.76 (17)
O1—C1—C2	106.7 (2)	N2—O14—Ca1	92.98 (17)
O1—C1—H1A	110.4	N2—O15—Ca1	99.68 (16)
C2—C1—H1A	110.4	N3—O17—Ca2	95.32 (16)
O1—C1—H1B	110.4	N3—O18—Ca2	93.17 (17)
C2—C1—H1B	110.4	N4—O20—Ca2	98.40 (16)
H1A—C1—H1B	108.6	N4—O21—Ca2	93.79 (16)

O15—Ca1—O1—C1	125.63 (19)	O20—Ca2—O9—C17	−74.1 (2)
O11—Ca1—O1—C1	67.77 (18)	O17—Ca2—O9—C17	−4.8 (3)
O12—Ca1—O1—C1	33.78 (19)	O8—Ca2—O9—C17	159.4 (2)
O4—Ca1—O1—C1	−138.30 (18)	O18—Ca2—O9—C17	−135.9 (2)
O3—Ca1—O1—C1	−71.37 (19)	O10—Ca2—O9—C17	−0.88 (19)
O5—Ca1—O1—C1	160.3 (2)	O6—Ca2—O9—C17	58.3 (2)
O2—Ca1—O1—C1	−19.12 (17)	O21—Ca2—O9—C17	−124.4 (2)
O14—Ca1—O1—C1	−144.1 (3)	O7—Ca2—O9—C17	121.2 (2)
N1—Ca1—O1—C1	52.18 (19)	O20—Ca2—O10—C19	−161.8 (2)
N2—Ca1—O1—C1	138.5 (2)	O17—Ca2—O10—C19	−78.76 (19)
O15—Ca1—O1—C10	−4.4 (2)	O8—Ca2—O10—C19	80.0 (2)
O11—Ca1—O1—C10	−62.28 (19)	O18—Ca2—O10—C19	−103.9 (2)
O12—Ca1—O1—C10	−96.28 (19)	O9—Ca2—O10—C19	103.15 (19)
O4—Ca1—O1—C10	91.65 (19)	O6—Ca2—O10—C19	−5.54 (18)
O3—Ca1—O1—C10	158.58 (18)	O21—Ca2—O10—C19	164.99 (18)
O5—Ca1—O1—C10	30.26 (18)	O7—Ca2—O10—C19	−6.4 (2)
O2—Ca1—O1—C10	−149.2 (2)	O20—Ca2—O10—C18	66.87 (17)
O14—Ca1—O1—C10	85.8 (4)	O17—Ca2—O10—C18	149.96 (18)
N1—Ca1—O1—C10	−77.87 (19)	O8—Ca2—O10—C18	−51.3 (2)
N2—Ca1—O1—C10	8.5 (3)	O18—Ca2—O10—C18	124.81 (18)
O15—Ca1—O2—C2	−142.67 (19)	O9—Ca2—O10—C18	−28.14 (17)
O11—Ca1—O2—C2	−94.66 (18)	O6—Ca2—O10—C18	−136.82 (19)
O12—Ca1—O2—C2	−147.90 (19)	O21—Ca2—O10—C18	33.70 (19)
O4—Ca1—O2—C2	63.27 (19)	O7—Ca2—O10—C18	−137.67 (17)
O3—Ca1—O2—C2	106.19 (19)	C10—O1—C1—C2	−178.9 (2)
O1—Ca1—O2—C2	−16.71 (17)	Ca1—O1—C1—C2	51.0 (3)
O5—Ca1—O2—C2	−17.4 (2)	C3—O2—C2—C1	176.9 (2)
O14—Ca1—O2—C2	151.63 (18)	Ca1—O2—C2—C1	47.8 (3)
N1—Ca1—O2—C2	−121.00 (19)	O1—C1—C2—O2	−63.6 (3)
N2—Ca1—O2—C2	177.50 (17)	C2—O2—C3—C4	−79.5 (3)
O15—Ca1—O2—C3	87.0 (2)	Ca1—O2—C3—C4	51.5 (3)

O11—Ca1—O2—C3	135.0 (2)	C5—O3—C4—C3	177.5 (2)
O12—Ca1—O2—C3	81.8 (2)	Ca1—O3—C4—C3	32.7 (3)
O4—Ca1—O2—C3	−67.1 (2)	O2—C3—C4—O3	−54.7 (4)
O3—Ca1—O2—C3	−24.14 (19)	C4—O3—C5—C6	−107.0 (3)
O1—Ca1—O2—C3	−147.0 (2)	Ca1—O3—C5—C6	39.9 (3)
O5—Ca1—O2—C3	−147.69 (19)	C7—O4—C6—C5	−168.0 (2)
O14—Ca1—O2—C3	21.3 (2)	Ca1—O4—C6—C5	47.8 (3)
N1—Ca1—O2—C3	108.7 (2)	O3—C5—C6—O4	−56.6 (3)
N2—Ca1—O2—C3	47.2 (2)	C6—O4—C7—C8	−171.8 (2)
O15—Ca1—O3—C4	−149.1 (2)	Ca1—O4—C7—C8	−29.7 (3)
O11—Ca1—O3—C4	−39.3 (3)	C9—O5—C8—C7	79.4 (3)
O12—Ca1—O3—C4	−73.0 (2)	Ca1—O5—C8—C7	−54.5 (3)
O4—Ca1—O3—C4	133.3 (2)	O4—C7—C8—O5	55.1 (3)
O1—Ca1—O3—C4	46.1 (2)	C8—O5—C9—C10	−162.0 (2)
O5—Ca1—O3—C4	115.3 (2)	Ca1—O5—C9—C10	−32.3 (3)
O2—Ca1—O3—C4	−5.7 (2)	C1—O1—C10—C9	169.6 (2)
O14—Ca1—O3—C4	−146.1 (2)	Ca1—O1—C10—C9	−59.0 (3)
N1—Ca1—O3—C4	−61.0 (2)	O5—C9—C10—O1	58.3 (3)
N2—Ca1—O3—C4	−146.4 (2)	C20—O6—C11—C12	177.5 (3)
O15—Ca1—O3—C5	66.5 (2)	Ca2—O6—C11—C12	−53.1 (3)
O11—Ca1—O3—C5	176.32 (18)	C13—O7—C12—C11	−172.3 (3)
O12—Ca1—O3—C5	142.61 (19)	Ca2—O7—C12—C11	−41.5 (3)
O4—Ca1—O3—C5	−11.02 (18)	O6—C11—C12—O7	60.7 (3)
O1—Ca1—O3—C5	−98.29 (19)	C12—O7—C13—C14	81.9 (3)
O5—Ca1—O3—C5	−29.1 (2)	Ca2—O7—C13—C14	−51.7 (3)
O2—Ca1—O3—C5	−150.1 (2)	C15—O8—C14—C13	177.6 (3)
O14—Ca1—O3—C5	69.54 (19)	Ca2—O8—C14—C13	−31.4 (4)
N1—Ca1—O3—C5	154.62 (18)	O7—C13—C14—O8	53.9 (4)
N2—Ca1—O3—C5	69.3 (2)	C14—O8—C15—C16	112.5 (3)
O15—Ca1—O4—C6	−144.81 (19)	Ca2—O8—C15—C16	−40.2 (3)
O11—Ca1—O4—C6	149.2 (2)	C17—O9—C16—C15	171.2 (2)
O12—Ca1—O4—C6	−81.5 (2)	Ca2—O9—C16—C15	−45.6 (3)
O3—Ca1—O4—C6	−20.82 (18)	O8—C15—C16—O9	55.1 (3)
O1—Ca1—O4—C6	84.35 (19)	C16—O9—C17—C18	168.9 (2)
O5—Ca1—O4—C6	144.3 (2)	Ca2—O9—C17—C18	27.7 (3)
O2—Ca1—O4—C6	21.5 (2)	C19—O10—C18—C17	−79.2 (3)
O14—Ca1—O4—C6	−96.92 (19)	Ca2—O10—C18—C17	55.3 (3)
N1—Ca1—O4—C6	−141.8 (3)	O9—C17—C18—O10	−53.8 (3)
N2—Ca1—O4—C6	−121.00 (19)	C18—O10—C19—C20	166.3 (2)
O15—Ca1—O4—C7	73.4 (2)	Ca2—O10—C19—C20	35.4 (3)
O11—Ca1—O4—C7	7.4 (3)	C11—O6—C20—C19	−173.9 (3)
O12—Ca1—O4—C7	136.7 (2)	Ca2—O6—C20—C19	55.5 (3)
O3—Ca1—O4—C7	−162.6 (2)	O10—C19—C20—O6	−58.7 (3)
O1—Ca1—O4—C7	−57.4 (2)	O13—N1—O11—Ca1	−176.4 (2)
O5—Ca1—O4—C7	2.51 (19)	O12—N1—O11—Ca1	4.0 (3)
O2—Ca1—O4—C7	−120.33 (19)	O15—Ca1—O11—N1	78.53 (16)
O14—Ca1—O4—C7	121.3 (2)	O12—Ca1—O11—N1	−2.28 (14)
N1—Ca1—O4—C7	76.4 (4)	O4—Ca1—O11—N1	148.06 (17)

N2—Ca1—O4—C7	97.2 (2)	O3—Ca1—O11—N1	−46.4 (2)
O15—Ca1—O5—C9	155.6 (2)	O1—Ca1—O11—N1	−142.84 (17)
O11—Ca1—O5—C9	78.07 (19)	O5—Ca1—O11—N1	152.58 (16)
O12—Ca1—O5—C9	105.08 (19)	O2—Ca1—O11—N1	−77.03 (16)
O4—Ca1—O5—C9	−104.24 (19)	O14—Ca1—O11—N1	44.16 (18)
O3—Ca1—O5—C9	−86.1 (2)	O13—N1—O12—Ca1	176.4 (2)
O1—Ca1—O5—C9	2.42 (17)	O11—N1—O12—Ca1	−4.0 (3)
O2—Ca1—O5—C9	3.1 (2)	O15—Ca1—O12—N1	−82.70 (16)
O14—Ca1—O5—C9	−167.10 (18)	O11—Ca1—O12—N1	2.29 (14)
N1—Ca1—O5—C9	90.52 (19)	O4—Ca1—O12—N1	−150.40 (15)
N2—Ca1—O5—C9	173.26 (18)	O3—Ca1—O12—N1	155.87 (15)
O15—Ca1—O5—C8	−73.51 (17)	O1—Ca1—O12—N1	45.37 (17)
O11—Ca1—O5—C8	−151.05 (17)	O5—Ca1—O12—N1	−32.6 (2)
O12—Ca1—O5—C8	−124.04 (17)	O2—Ca1—O12—N1	94.36 (16)
O4—Ca1—O5—C8	26.63 (16)	O14—Ca1—O12—N1	−135.08 (16)
O3—Ca1—O5—C8	44.8 (2)	O16—N2—O14—Ca1	−173.9 (2)
O1—Ca1—O5—C8	133.30 (18)	O15—N2—O14—Ca1	4.5 (2)
O2—Ca1—O5—C8	133.96 (17)	O15—Ca1—O14—N2	−2.72 (15)
O14—Ca1—O5—C8	−36.22 (18)	O11—Ca1—O14—N2	42.63 (18)
N1—Ca1—O5—C8	−138.60 (17)	O12—Ca1—O14—N2	78.85 (16)
N2—Ca1—O5—C8	−55.86 (17)	O4—Ca1—O14—N2	−109.13 (16)
O20—Ca2—O6—C20	4.4 (2)	O3—Ca1—O14—N2	−179.41 (17)
O17—Ca2—O6—C20	66.09 (18)	O1—Ca1—O14—N2	−103.1 (3)
O8—Ca2—O6—C20	−153.80 (18)	O5—Ca1—O14—N2	−51.48 (17)
O18—Ca2—O6—C20	100.27 (19)	O2—Ca1—O14—N2	137.54 (15)
O9—Ca2—O6—C20	−87.03 (18)	O16—N2—O15—Ca1	173.6 (2)
O10—Ca2—O6—C20	−27.06 (17)	O14—N2—O15—Ca1	−4.8 (3)
O7—Ca2—O6—C20	152.2 (2)	O11—Ca1—O15—N2	−135.74 (18)
O20—Ca2—O6—C11	−124.99 (18)	O12—Ca1—O15—N2	−81.66 (17)
O17—Ca2—O6—C11	−63.34 (18)	O4—Ca1—O15—N2	70.38 (17)
O8—Ca2—O6—C11	76.76 (18)	O3—Ca1—O15—N2	6.4 (2)
O18—Ca2—O6—C11	−29.16 (19)	O1—Ca1—O15—N2	167.03 (15)
O9—Ca2—O6—C11	143.54 (17)	O5—Ca1—O15—N2	134.68 (18)
O10—Ca2—O6—C11	−156.49 (19)	O2—Ca1—O15—N2	−86.8 (2)
O7—Ca2—O6—C11	22.77 (17)	O14—Ca1—O15—N2	2.74 (15)
O20—Ca2—O7—C13	−86.4 (2)	O19—N3—O17—Ca2	−166.3 (2)
O17—Ca2—O7—C13	−140.5 (2)	O18—N3—O17—Ca2	14.3 (3)
O8—Ca2—O7—C13	24.2 (2)	O20—Ca2—O17—N3	−90.30 (16)
O18—Ca2—O7—C13	−87.3 (2)	O8—Ca2—O17—N3	42.5 (2)
O9—Ca2—O7—C13	63.0 (2)	O18—Ca2—O17—N3	−8.11 (15)
O10—Ca2—O7—C13	144.2 (2)	O9—Ca2—O17—N3	−160.95 (16)
O6—Ca2—O7—C13	143.4 (2)	O10—Ca2—O17—N3	−164.52 (16)
O21—Ca2—O7—C13	−26.8 (2)	O6—Ca2—O17—N3	130.71 (17)
O20—Ca2—O7—C12	141.49 (19)	O21—Ca2—O17—N3	−50.97 (17)
O17—Ca2—O7—C12	87.35 (19)	O7—Ca2—O17—N3	64.72 (16)
O8—Ca2—O7—C12	−107.9 (2)	O19—N3—O18—Ca2	166.6 (2)
O18—Ca2—O7—C12	140.6 (2)	O17—N3—O18—Ca2	−14.0 (2)
O9—Ca2—O7—C12	−69.1 (2)	O20—Ca2—O18—N3	96.67 (16)

O10—Ca2—O7—C12	12.1 (2)	O17—Ca2—O18—N3	8.13 (15)
O6—Ca2—O7—C12	11.24 (18)	O8—Ca2—O18—N3	−142.44 (16)
O21—Ca2—O7—C12	−158.94 (18)	O9—Ca2—O18—N3	160.52 (15)
O20—Ca2—O8—C14	150.6 (2)	O10—Ca2—O18—N3	40.7 (2)
O17—Ca2—O8—C14	29.6 (3)	O6—Ca2—O18—N3	−34.88 (17)
O18—Ca2—O8—C14	67.7 (2)	O21—Ca2—O18—N3	148.93 (17)
O9—Ca2—O8—C14	−138.3 (3)	O7—Ca2—O18—N3	−83.82 (16)
O10—Ca2—O8—C14	−115.3 (2)	O22—N4—O20—Ca2	−172.0 (2)
O6—Ca2—O8—C14	−48.2 (2)	O21—N4—O20—Ca2	7.5 (2)
O21—Ca2—O8—C14	138.9 (3)	O17—Ca2—O20—N4	128.48 (17)
O7—Ca2—O8—C14	5.3 (2)	O8—Ca2—O20—N4	−18.66 (19)
O20—Ca2—O8—C15	−59.0 (2)	O18—Ca2—O20—N4	75.86 (16)
O17—Ca2—O8—C15	179.98 (19)	O9—Ca2—O20—N4	−78.75 (16)
O18—Ca2—O8—C15	−141.9 (2)	O10—Ca2—O20—N4	−143.95 (17)
O9—Ca2—O8—C15	12.1 (2)	O6—Ca2—O20—N4	−173.39 (14)
O10—Ca2—O8—C15	35.1 (2)	O21—Ca2—O20—N4	−4.31 (14)
O6—Ca2—O8—C15	102.2 (2)	O7—Ca2—O20—N4	75.0 (2)
O21—Ca2—O8—C15	−70.7 (2)	O22—N4—O21—Ca2	172.3 (2)
O7—Ca2—O8—C15	155.7 (2)	O20—N4—O21—Ca2	−7.2 (2)
O20—Ca2—O9—C16	145.57 (19)	O20—Ca2—O21—N4	4.30 (14)
O17—Ca2—O9—C16	−145.16 (19)	O17—Ca2—O21—N4	−49.60 (17)
O8—Ca2—O9—C16	19.05 (18)	O8—Ca2—O21—N4	171.53 (17)
O18—Ca2—O9—C16	83.7 (2)	O18—Ca2—O21—N4	−83.19 (16)
O10—Ca2—O9—C16	−141.2 (2)	O9—Ca2—O21—N4	102.47 (16)
O6—Ca2—O9—C16	−82.07 (19)	O10—Ca2—O21—N4	46.84 (17)
O21—Ca2—O9—C16	95.24 (18)	O7—Ca2—O21—N4	−140.76 (15)
O7—Ca2—O9—C16	−19.2 (2)		