JOURNAL OF SOLID STATE CHEMISTRY 50, 240–246 (1983)

Crystal Structure of Cerium(III) Diammonium Polyphosphate $(NH_4)_2Ce(PO_3)_5$

M. RZAIGUI AND KBIR ARIGUIB

Laboratoire de Physico-Chemie Minérale, Ecole Normale Supérieure, 43, Rue de la liberté, Le Bardo, Tunis

AND M. T. AVERBUCH-POUCHOT AND A. DURIF

Laboratoire de Cristallographie, CNRS, Laboratoire associé à l'USMG, 166X Centre de tri, 38042 Grenoble Cedex, France

Received January 4, 1983; in revised form July 15, 1983

Cerium(III) diammonium polyphosphate, $(NH_4)_2Ce(PO_3)_5$, is triclinic $P\bar{1}$ with the following unit cell dimensions: a = 7.241(5) Å, b = 13.314(8) Å, c = 7.241(5) Å, α = 90.35(5)°, β' = 107.50(5)°, γ = 90.28(5)°, and Z = 2, V = 665.7 Å^3, D_x = 2.85 g/cm^3. The crystal structure of this new type of polyphosphate has been solved and refined from 4130 independent reflections to a final R value 0.029. The most interesting feature of this salt is the existence of two infinite crystallographically nonequivalent $(PO_3)_\infty^-$ chains, one running parallel to the a axis, the other along the c axis, both with a period of five tetrahedra. This compound seems to be the first example of a long chain polyphosphate with crystallographic independent chains.

Introduction

$Ce(PO_3)_3$–M^IPO_3, with M^I = Li, Na, K, phase diagrams have been investigated (*1*, *2*). One of them, for M^I = K, shows the formation of $M^I_2Ce(PO_3)_5$ compounds. The crystalline structures of this type of compound have not yet been investigated. The present work reports the crystal structure of $(NH_4)_2Ce(PO_3)_5$.

Experimental

Chemical Preparation and Crystal Chemistry

The preparation of this compound has already been published (*3*). The crystals are usually thick diamond-like plates.

From the first investigations by film techniques, the unit cell seemed to be monoclinic, with

$$a = 7.224 \text{ Å}, \quad b = 13.31 \text{ Å}, \quad c = 7.24 \text{ Å}, \quad \beta = 107.5°$$

or possibly orthorhombic, with

$$\mathbf{a} = \frac{a + c}{2}, \qquad \mathbf{b} = b, \qquad \mathbf{c} = \frac{a - c}{2}.$$

However, a closer inspection of the intensity of reflections showed that these two possibilities were incorrect. The unit cell is, in fact, triclinic in spite of its unusual dimensions. Refinement of data from a four circle diffractometer show the dimensions of this unit cell to be

0022-4596/83 $3.00

TABLE I

MEASUREMENT PARAMETERS USED FOR THE X-RAY DIFFRACTION DATA COLLECTION

Apparatus:	Philips PW 1100	Total back ground time measurement:	10 sec
Wavelength:	AgKα (0.5608 Å)	Scan width:	1.20°
Monochromator:	Graphite plate	Intensity reflections:	0 10 0 and 0 $\bar{1}\bar{0}$ 0
Scan mode:	ω	Number of collected reflections:	4764 ($\pm H$, $\pm K$, L)
Angular domain:	3–25°(θ)	Crystal size:	0.16 × 0.16 × 0.13 mm³
Scan speed:	0.03°/sec		

$a = 7.241(5)$ Å, $b = 13.314(8)$ Å, $c = 7.241(5)$ Å

$\alpha = 90.35(5)°$, $\beta = 107.50(5)°$, $\gamma = 90.28(5)°$

with $Z = 2$, $V = 665.7$ Å^3, and $D_x = 2.850$ g/cm^3. From positive piezoelectric tests the space group $P1$ was assumed and later confirmed by the structure determination.

Structure Determination

Table I reports the experimental conditions used for the data collection. The crystal structure was solved by using classical methods: interpretation of three-dimensional Patterson maps followed by successive Fourier syntheses. After a few refinement cycles using anisotropic thermal parameters the final R value was 0.029 for a

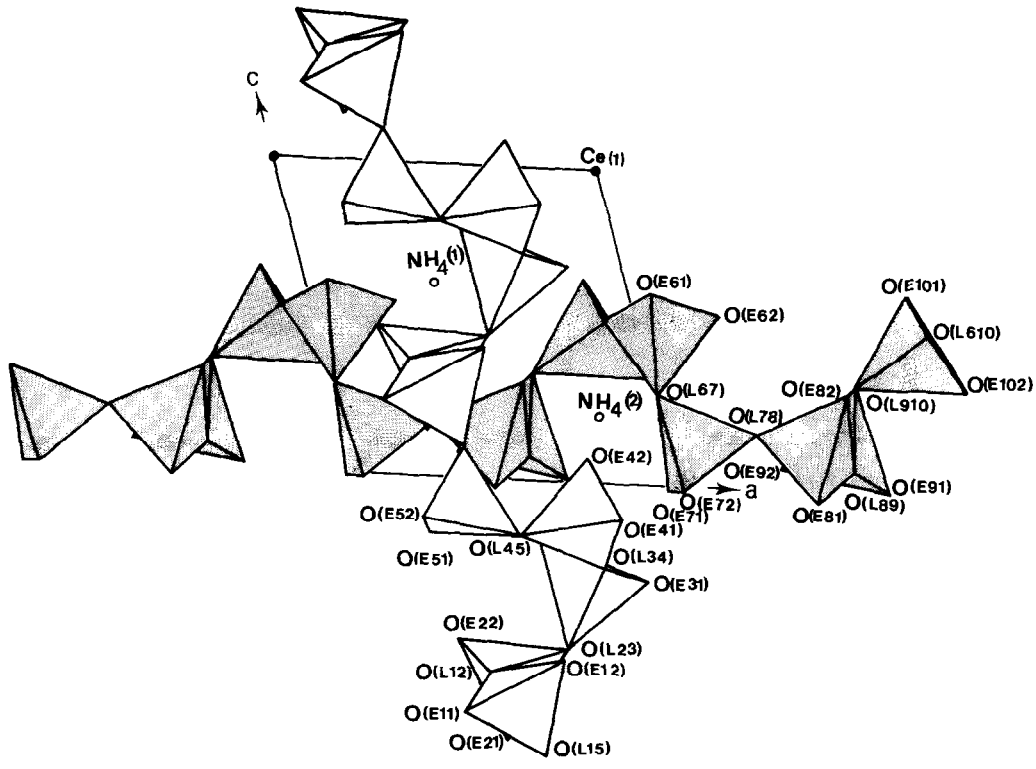

FIG. 1. Projection of the atomic arrangement of $(NH_4)_2Ce(PO_3)_5$ along the b axis. PO_4 tetrahedra of the chain running along the a axis shaded.

TABLE II

FINAL ATOMIC COORDINATES AND EQUIVALENT TEMPERATURE FACTORS ($B_{eq.}$)

Atoms	$X(\sigma)$	$Y(\sigma)$	$Z(\sigma)$	$B_{eq.}$ (σ)
Ce(1)	0.00000(0)	0.00000(0)	0.00000(0)	0.621(3)
Ce(2)	0.19107(6)	0.50004(3)	0.80890(6)	0.628(4)
P(1)	0.3243(3)	0.8065(1)	0.2887(3)	0.80(3)
P(2)	0.3030(3)	0.5890(1)	0.3564(3)	0.79(3)
P(3)	0.6562(3)	0.5778(1)	0.6797(3)	0.86(3)
P(4)	0.6942(3)	0.7633(1)	0.8979(3)	0.94(3)
P(5)	0.2798(3)	0.7809(1)	0.8761(3)	0.79(3)
P(6)	0.0855(3)	0.2631(1)	0.5062(3)	0.93(3)
P(7)	0.0642(3)	0.2809(1)	0.0925(3)	0.75(3)
P(8)	0.4769(3)	0.3067(1)	0.1365(3)	0.84(3)
P(9)	0.5430(3)	0.0893(1)	0.1153(3)	0.79(3)
P(10)	0.8676(3)	0.0777(1)	0.4686(3)	0.83(3)
O(L12)	0.2605(8)	0.7054(4)	0.3724(8)	1.25(9)
O(L15)	0.3676(9)	0.7653(5)	0.1014(8)	1.47(10)
O(E11)	0.1505(8)	0.8730(4)	0.2402(8)	1.31(9)
O(E12)	0.5054(9)	0.8478(5)	0.4223(10)	1.84(11)
O(L23)	0.5316(8)	0.5818(5)	0.4567(8)	1.23(9)
O(E21)	0.2662(9)	0.5582(5)	0.1515(8)	1.49(10)
O(E22)	0.1947(8)	0.5384(5)	0.4745(8)	1.38(9)
O(L34)	0.7094(9)	0.6925(4)	0.7249(8)	1.48(10)
O(E31)	0.8381(9)	0.5273(5)	0.6864(10)	1.70(10)
O(E32)	0.5347(9)	0.5395(5)	0.7972(9)	1.55(10)
O(L45)	0.4719(8)	0.7918(5)	0.8181(8)	1.60(10)
O(E41)	0.8012(9)	0.8553(5)	0.8865(10)	1.76(10)
O(E42)	0.7429(10)	0.7074(5)	0.0808(9)	1.65(10)
O(E51)	0.1753(10)	0.6889(5)	0.7897(10)	1.79(10)
O(E52)	0.1778(8)	0.8795(5)	0.8321(9)	1.45(10)
O(L67)	0.0050(9)	0.2909(6)	0.2841(8)	1.87(12)
O(L610)	0.9113(8)	0.1921(4)	0.5233(9)	1.41(9)
O(E61)	0.0733(10)	0.3557(5)	0.6145(9)	1.69(10)
O(E62)	0.2679(9)	0.2079(5)	0.5544(10)	1.75(11)
O(L78)	0.2898(8)	0.2666(5)	0.1812(9)	1.38(9)
O(E71)	0.9765(9)	0.1876(5)	0.9896(10)	1.66(10)
O(E72)	0.0201(8)	0.3779(4)	−0.0079(8)	1.21(9)
O(L89)	0.5627(8)	0.2045(4)	0.0750(9)	1.33(9)
O(E81)	0.4271(9)	0.3721(5)	0.9638(9)	1.44(9)
O(E82)	0.6101(10)	0.3481(5)	0.3192(10)	1.76(11)
O(L910)	0.6440(8)	0.0815(5)	0.3441(8)	1.24(9)
O(E91)	0.6612(8)	0.0383(5)	0.0087(9)	1.34(9)
O(E92)	0.3405(8)	0.0582(5)	0.0808(10)	1.62(10)
O(E101)	0.8735(11)	0.0255(5)	0.6511(9)	1.83(11)
O(E102)	0.9848(9)	0.0398(5)	0.3485(9)	1.51(10)
N(1)	0.4000(1)	0.0065(6)	0.625(1)	1.79(13)
N(2)	0.812(1)	0.5080(7)	0.215(1)	2.34(15)
N(3)	0.883(1)	0.8017(7)	0.456(1)	1.89(13)
N(4)	0.647(1)	0.3008(8)	0.699(1)	2.13(15)

Notes. $B_{eq.} = \frac{4}{3} \Sigma_i \Sigma_j \, a_i \cdot a_j \cdot \beta_{ij}$. The notation adopted for atoms is the present accepted system for condensed anions: an oxygen atom connecting two phosphorus atoms P(*i*) and P(*j*) will be denoted O(L*ij*) while the two external oxygen atoms of a given P(*i*) will be denoted O(E*i*1) and O(E*i*2).

set of 4130 independent reflections fulfilling to the criterion $F_0 > 2\sigma_F$. In the refinements unitary weights were always used. Lorentz and polarization corrections have been made; however, due to the small crystal size and the short wavelength, no absorption correction was applied (μ = 21.5 cm^{-1}).

Table II gives the final atomic coordinates and the equivalent temperature factors, while the anisotropic thermal parameters are listed on Table III. A table of structure factors is available from the authors.

Structure Description

This compound is a long chain polyphosphate. The main feature of this atomic arrangement is the existance of two independent $(PO_3)_\infty$ chains, one running along the *a* axis, the other along the *c* axis (Fig. 1).

Chain 1, involving phosphorus atoms P(1) to P(5), runs parallel to *c* axis with a period of five tetrahedra (Fig. 2). Interatomic distances and bond angles in one period of this chain are given in Table IV. The average P–O bond lengths are 1.538, 1.539, 1.553, 1.529, and 1.530 Å, respectively, for $P(1)O_4$ to $P(5)O_4$, while the P–O(L)–P angles are in the range from 131.1 to 139.6°.

Chain 2, with detailed data concerning interatomic distances and bond angles reported in Table V, runs parallel to the *a* axis (Fig. 3). Its periodicity is also five tetrahedra and involves the phosphorus P(6) to P(10). The P–O average values are 1.532, 1.528, 1.539, 1.531, and 1.534 Å.

From these data, it appears that the main features of these phosphate chains are not significantly different from what is commonly observed in classical chain polyphosphates.

Associated cations. Cerium atoms have an eightfold coordination with Ce–O distances ranging from 2.387 to 2.579 Å for Ce(1), and from 2.373 to 2.633 Å for Ce(2). Attempts to find noncrystallographic symmetry in these polyhedra have failed. Table VI reports Ce–O distances within these polyhedra.

TABLE III

ANISOTROPIC THERMAL PARAMETERS (THERMAL FACTOR IS $T = h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + hk\beta_{12} + hl\beta_{13} + kl\beta_{23}$)

Atoms	$\beta(1,1)$ (σ)	$\beta(2,2)$ (σ)	$\beta(3,3)$ (σ)	$\beta(1,2)$ (σ)	$\beta(1,3)$ (σ)	$\beta(2,3)$ (σ)
Ce(1)	0.00321(4)	0.00070(1)	0.00373(5)	−0.00016(4)	0.00145(8)	0.00021(4)
Ce(2)	0.00356(4)	0.00081(1)	0.00320(5)	0.00020(4)	0.00175(7)	−0.00007(4)
P(1)	0.0048(2)	0.00102(7)	0.0042(3)	0.0007(2)	0.0031(4)	0.0000(2)
P(2)	0.0045(2)	0.00121(7)	0.0033(3)	−0.0005(2)	0.0020(4)	0.0000(2)
P(3)	0.0038(2)	0.00107(7)	0.0053(7)	−0.0001(2)	0.0018(4)	0.0004(3)
P(4)	0.0042(2)	0.00118(8)	0.0058(3)	−0.0005(2)	0.0020(4)	−0.0008(3)
P(5)	0.0042(2)	0.00123(7)	0.0039(3)	0.0002(2)	0.0031(4)	−0.0003(3)
P(6)	0.0065(3)	0.00117(7)	0.0038(3)	−0.0008(2)	0.0033(4)	0.0000(3)
P(7)	0.0044(2)	0.00085(7)	0.0045(3)	−0.0010(2)	0.0035(4)	−0.0002(2)
P(8)	0.0039(2)	0.00092(7)	0.0060(3)	0.0001(2)	0.0038(4)	0.0003(3)
P(9)	0.0032(2)	0.00096(7)	0.0052(3)	−0.0002(2)	0.0013(4)	−0.0006(3)
P(10)	0.0055(3)	0.00087(7)	0.0040(3)	0.0009(2)	0.0016(4)	0.0004(2)
O(L12)	0.0084(8)	0.0013(2)	0.0083(9)	0.0025(7)	0.010(1)	0.0008(8)
O(L15)	0.0105(9)	0.0024(3)	0.0052(8)	0.0045(9)	0.009(1)	0.0021(8)
O(E11)	0.0083(8)	0.0019(2)	0.0062(8)	0.0054(8)	0.007(1)	0.0028(8)
O(E12)	0.0073(10)	0.0029(3)	0.0094(11)	−0.0019(10)	0.000(2)	−0.0030(11)
O(L23)	0.0057(8)	0.0026(3)	0.0042(8)	−0.0003(8)	0.004(1)	0.0007(9)
O(E21)	0.0116(11)	0.0020(3)	0.0044(8)	−0.0031(9)	0.005(2)	−0.0014(8)
O(E22)	0.0078(9)	0.0021(3)	0.0063(9)	−0.0037(8)	0.004(1)	0.0017(8)
O(L34)	0.0130(10)	0.0013(2)	0.0078(9)	−0.0015(8)	0.013(1)	−0.0019(8)
O(E31)	0.0059(9)	0.0018(3)	0.0127(12)	0.0022(8)	0.001(2)	−0.0018(10)
O(E32)	0.0092(10)	0.0022(3)	0.0065(9)	−0.0024(9)	0.003(2)	0.0030(9)
O(L45)	0.0037(7)	0.0040(3)	0.0065(9)	0.0035(9)	0.003(1)	0.057(10)
O(E41)	0.0090(10)	0.0015(3)	0.0123(12)	−0.0039(8)	0.004(2)	−0.0027(10)
O(E42)	0.0097(11)	0.0024(3)	0.0060(10)	0.0009(10)	0.000(2)	−0.0001(10)
O(E51)	0.0119(11)	0.0017(3)	0.0085(11)	−0.0019(10)	0.002(2)	−0.0030(10)
O(E52)	0.0083(9)	0.0018(3)	0.0093(10)	0.0022(8)	0.009(1)	0.0024(9)
O(L67)	0.0080(9)	0.0047(4)	0.0046(9)	0.0051(10)	0.005(1)	0.0030(10)
O(L610)	0.0090(9)	0.0009(2)	0.0116(10)	−0.0013(8)	0.012(1)	−0.0008(8)
O(E61)	0.0122(11)	0.0014(2)	0.0096(10)	−0.0024(9)	0.008(2)	−0.0036(9)
O(E62)	0.0074(10)	0.0026(3)	0.0097(11)	0.0014(9)	0.002(2)	0.0024(10)
O(L78)	0.0057(8)	0.0021(3)	0.0089(9)	0.0000(8)	0.006(1)	0.0035(9)
O(E71)	0.0080(10)	0.0014(2)	0.0112(12)	−0.0016(9)	0.000(2)	−0.0010(10)
O(E72)	0.0088(9)	0.0011(2)	0.0063(9)	0.0008(8)	0.005(1)	0.0024(8)
O(L89)	0.0069(8)	0.0014(2)	0.0112(10)	0.0015(7)	0.012(1)	0.0010(8)
O(E81)	0.0086(9)	0.0019(3)	0.0078(9)	0.0034(8)	0.007(1)	0.0044(9)
O(E82)	0.0099(11)	0.0020(3)	0.0091(11)	−0.0020(9)	0.002(2)	−0.0009(10)
O(L910)	0.0070(9)	0.0023(3)	0.0035(8)	0.0007(8)	0.001(1)	0.0017(8)
O(E91)	0.0057(8)	0.0019(2)	0.0082(10)	0.0018(8)	0.004(1)	−0.0036(9)
O(E92)	0.0047(8)	0.0019(3)	0.0122(12)	−0.0011(8)	0.001(2)	−0.0009(10)
O(E101)	0.0156(13)	0.0017(3)	0.0059(10)	−0.0005(10)	0.003(2)	0.0022(9)
O(E102)	0.0080(9)	0.0024(3)	0.0067(9)	0.0013(9)	0.004(2)	−0.0032(9)
N(1)	0.009(1)	0.0031(4)	0.007(1)	0.000(1)	0.000(2)	−0.001(1)
N(2)	0.014(2)	0.0025(4)	0.012(2)	−0.003(1)	0.004(3)	0.000(1)
N(3)	0.007(1)	0.0036(4)	0.010(1)	0.001(1)	0.006(2)	0.004(1)
N(4)	0.008(1)	0.0047(5)	0.010(1)	0.001(1)	0.011(2)	−0.002(1)

TABLE IV

MAIN INTERATOMIC DISTANCES (Å) AND BOND ANGLES (°) IN CHAIN 1

P(1)O_4 tetrahedron				
P(1)	O(L12)	O(L15)	O(E11)	O(E12)
O(L12)	1.601(6)	2.453(7)	2.472(7)	2.538(8)
O(L15)	101.0(3)	1.577(5)	2.548(6)	2.484(8)
O(E11)	105.9(3)	112.0(3)	1.497(5)	2.536(7)
O(E12)	111.0(3)	108.8(3)	117.0(3)	1.478(5)

P(2)O tetrahedron				
P(2)	O(L12)	O(L23)	O(E21)	O(E22)
O(L12)	1.591(6)	2.501(7)	2.530(7)	2.437(7)
O(L23)	103.3(3)	1.599(5)	2.471(7)	2.545(7)
O(E21)	110.8(3)	106.6(3)	1.481(5)	2.557(7)
O(E22)	104.8(3)	111.2(3)	119.1(3)	1.485(5)

P(3)O_4 tetrahedron				
P(3)	O(L23)	O(L34)	O(E31)	O(E32)
O(L23)	1.597(5)	2.459(7)	2.456(7)	2.527(7)
O(L34)	101.3(3)	1.581(5)	2.440(7)	2.533(7)
O(E31)	106.3(3)	106.1(3)	1.470(5)	2.561(8)
O(E32)	110.0(3)	111.3(3)	120.1(3)	1.486(5)

P(4)O_4 tetrahedron				
P(4)	O(L34)	O(L45)	O(E41)	O(E42)
O(L34)	1.594(5)	2.423(7)	2.449(7)	2.522(8)
O(L45)	99.2(3)	1.587(5)	2.432(7)	2.557(8)
O(E41)	106.4(3)	105.7(3)	1.463(5)	2.535(8)
O(E42)	110.6(3)	113.4(3)	119.4(3)	1.472(6)

P(5)O_4 tetrahedron				
P(5)	O(L15)	O(L45)	O(E51)	O(E52)
O(L15)	1.578(5)	2.417(7)	2.476(8)	2.539(7)
O(L45)	100.1(3)	1.576(5)	2.496(8)	2.462(7)
O(E51)	108.6(3)	110.1(3)	1.469(6)	2.552(7)
O(E52)	111.3(3)	106.4(3)	118.7(3)	1.497(5)

Other distances and bond angles of interest in the chain

P(1)–P(2)	2.950(2)	P(1)–O(L12)–P(2)	135.1(4)
P(2)–P(3)	2.907(2)	P(2)–O(L23)–P(3)	130.9(4)
P(3)–P(4)	2.891(2)	P(3)–O(L34)–P(4)	131.1(4)
P(4)–P(5)	2.967(2)	P(4)–O(L45)–P(5)	139.6(4)
P(5)–P(1)	2.924(2)	P(5)–O(L15)–P(1)	135.9(4)

TABLE V

MAIN INTERATOMIC DISTANCES (Å) AND BOND ANGLES (°) IN CHAIN 2

P(6)O_4 tetrahedron				
P(6)	O(L67)	O(L610)	O(E61)	O(E62)
O(L67)	1.584(6)	2.433(8)	2.444(8)	2.546(8)
O(L610)	99.3(3)	1.608(5)	2.460(7)	2.531(8)
O(E61)	106.0(3)	105.8(3)	1.474(5)	2.536(8)
O(E62)	113.3(3)	110.9(3)	119.4(3)	1.463(6)

P(7)O_4 tetrahedron				
P(7)	O(L67)	O(L78)	O(E71)	O(E72)
O(L67)	1.575(6)	2.417(7)	2.486(8)	2.447(7)
O(L78)	100.0(3)	1.579(5)	2.499(7)	2.516(7)
O(E71)	108.7(3)	109.4(3)	1.482(5)	2.551(7)
O(E72)	106.7(3)	110.9(3)	119.2(3)	1.475(5)

P(8)O_4 tetrahedron				
P(8)	O(L78)	O(L89)	O(E81)	O(E82)
O(L78)	1.576(5)	2.470(7)	2.529(7)	2.475(7)
O(L89)	101.5(3)	1.614(6)	2.483(7)	2.547(8)
O(E81)	111.5(3)	106.5(3)	1.483(5)	2.539(8)
O(E82)	107.9(3)	110.5(3)	117.7(3)	1.484(6)

P(9)O_4 tetrahedron				
P(9)	O(L89)	O(L910)	O(E91)	O(E92)
O(L89)	1.576(6)	2.486(7)	2.417(7)	2.529(8)
O(L910)	102.9(3)	1.602(5)	2.532(7)	2.455(7)
O(E91)	104.5(3)	110.5(3)	1.478(5)	2.543(7)
O(E92)	112.2(3)	106.1(3)	119.3(3)	1.469(5)

P(10)O_4 tetrahedron				
P(10)	O(L610)	O(L910)	O(E101)	O(E102)
O(L610)	1.577(5)	2.457(7)	2.454(7)	2.525(7)
O(L910)	101.3(3)	1.600(5)	2.464(7)	2.523(7)
O(E101)	106.4(3)	105.9(3)	1.486(5)	2.560(8)
O(E102)	111.7(3)	110.2(3)	119.7(3)	1.475(5)

Other distances and bond angles of interest in the chain

P(6) –P(7)	2.964(2)	P(6) –O(L67) –P(7)	139.4(4)
P(7) –P(8)	2.927(2)	P(7) –O(L78) –P(8)	136.2(4)
P(8) –P(9)	2.946(2)	P(8) –O(L89) –P(9)	134.9(4)
P(9) –P(10)	2.913(2)	P(9) –O(L910)–P(10)	131.0(4)
P(10)–P(6)	2.890(2)	P(10)–O(L106)–P(6)	130.3(4)

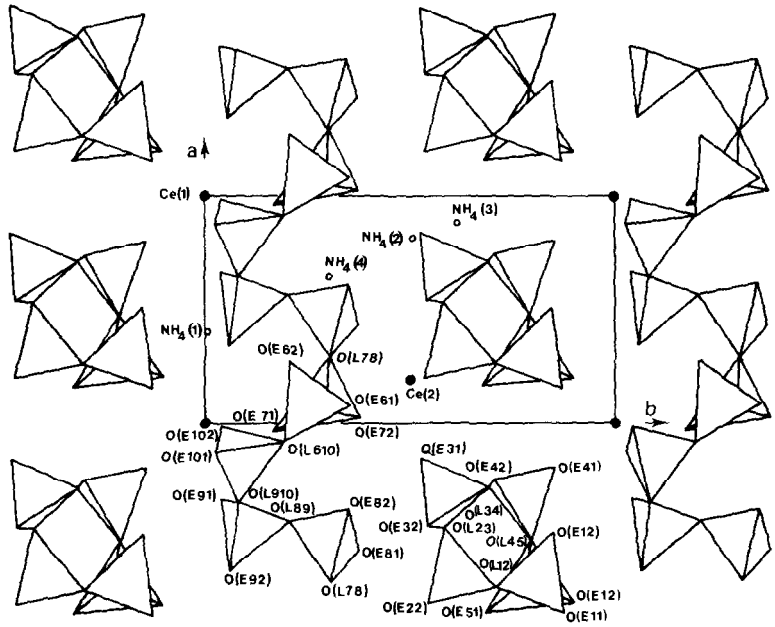

FIG. 2. Projection of the atomic arrangement of $(NH_4)_2Ce(PO_3)_5$ along the c axis.

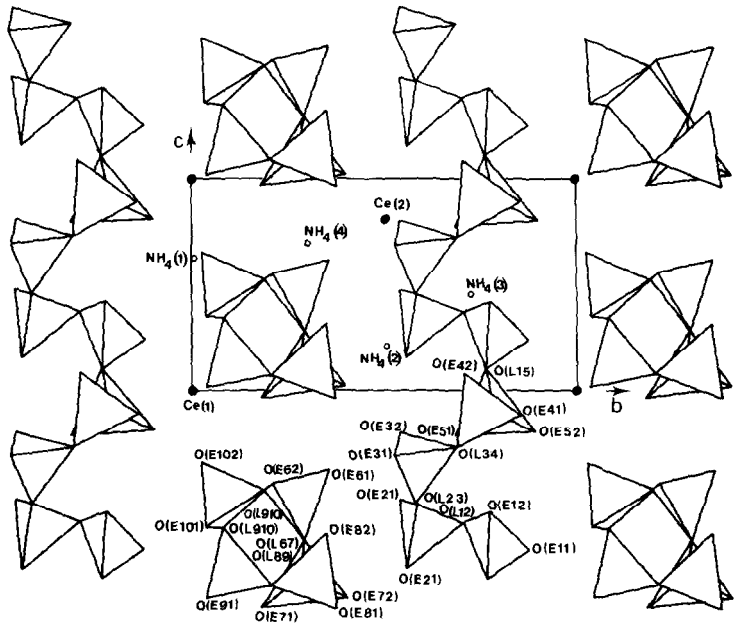

FIG. 3. Projection of the atomic arrangement of $(NH_4)_2Ce(PO_3)_5$ along the a axis.

TABLE VI

CERIUM–OXYGEN DISTANCES IN THE CeO_8 POLYHEDRA (Å)

Ce(1)–O(E11)	2.447(5)	Ce(1)–O(E91)	2.527(5)
Ce(1)–O(E41)	2.587(5)	Ce(1)–O(E92)	2.476(5)
Ce(1)–O(E52)	2.579(5)	Ce(1)–O(E101)	2.441(5)
Ce(1)–O(E71)	2.504(5)	Ce(1)–O(E102)	2.610(5)
$Ce(2)O_8$ polyhedron			
Ce(2)–O(E21)	2.492(5)	Ce(2)–O(E51)	2.521(5)
Ce(2)–O(E22)	2.486(5)	Ce(2)–O(E61)	2.373(5)
Ce(2)–O(E31)	2.470(5)	Ce(2)–O(E72)	2.633(5)
Ce(2)–O(E32)	2.567(5)	Ce(2)–O(E81)	2.445(5)

Ammonium groups. If limited to a maximum distance of 3.5 Å the N–O distances correspond to NO_9 polyhedra for N(1) and N(2) and NO_{10} polyhedra for N(3) and N(4). Noncrystallographic symmetry for these polyhedra could not be detected. Table VII reports all N–O distances in these coordination polyhedra. Due to the presence of an heavy atom (Ce), hydrogen atoms have not been located.

TABLE VII

NITROGEN–OXYGEN DISTANCES IN THE NO_9 AND NO_{10} POLYHEDRA (Å)

N(1)–O(E11)	3.327(10)	N(2)–O(L23)	3.204(12)
N(1)–O(E12)	2.800(11)	N(2)–O(E22)	2.869(11)
N(1)–O(L45)	3.166(11)	N(2)–O(E31)	3.367(12)
N(1)–O(E52)	3.028(11)	N(2)–O(E32)	3.119(11)
N(1)–O(E62)	2.849(11)	N(2)–O(E42)	2.827(12)
N(1)–O(L910)	3.226(11)	N(2)–O(L67)	3.194(12)
N(1)–O(E91)	2.880(10)	N(2)–O(E72)	3.057(12)
N(1)–O(E101)	3.382(11)	N(2)–O(E81)	3.347(11)
N(1)–O(E102)	3.107(10)	N(2)–O(E82)	2.807(11)
$N(3)O_4$ polyhedron		$N(4)O_{10}$ polyhedron	
N(3)–O(L12)	3.241(10)	N(4)–O(E31)	3.325(11)
N(3)–O(E11)	2.986(9)	N(4)–O(E32)	3.408(11)
N(3)–O(E12)	2.743(9)	N(4)–O(L610)	2.973(9)
N(3)–O(L34)	2.995(9)	N(4)–O(E61)	3.399(10)
N(3)–O(E41)	3.416(10)	N(4)–O(E62)	2.895(11)
N(3)–O(E42)	2.875(11)	N(4)–O(E71)	3.074(11)
N(3)–O(E51)	3.095(10)	N(4)–O(E72)	3.060(11)
N(3)–O(E52)	3.083(10)	N(4)–O(L89)	3.237(10)
N(3)–O(E101)	3.300(11)	N(4)–O(E81)	2.992(9)
N(3)–O(E102)	3.400(10)	N(4)–O(E82)	2.757(11)

The present structure determination can probably clarify a recent work of Palkina *et al.* (*4*) describing the crystal structure of a cerium–ammonium polyphosphate with an uncertain formula. The compound described by these authors is probably $NH_4Ce^{IV}(PO_3)_5$ or $NH_4CeH(PO_3)_5$. Besides the title compound, we have also observed the existence of $K_2Ce(PO_3)_5$, $Rb_2Ce(PO_3)_5$, $Cs_2Ce(PO_3)_5$, $Tl_2Ce(PO_3)_5$, and Nd-containing analogs. Crystallographic data of the latter will be given in subsequent contributions. These compounds are the first examples of condensed phosphates with such a formula and to the present the first evidence for the existence of crystallographic independent infinite PO_4 chains.

References

1. M. RZAIGUI AND N. K. ARIGUIB, *J. Solid State Chem.* **39**, 309 (1981).
2. M. RZAIGUI, M. DABBABI, AND N. K. ARIGUIB, *J. Chim. Phys.* **6**, (78), 563 (1981).
3. M. RZAIGUI AND N. K. ARIGUIB, to be published.
4. K. K. PALKINA, V. V. KRASNIKOV, AND Z. A. KONSTANT, *Izv. Akad. Nauk SSSR, Neorg. Mater.* **17** (7), 1243 (1981).