Research Article

$\text{Na}_3\text{MP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$ ($\text{M} = \text{Co}, \text{Ni}$): Crystal Structure and IR Spectroscopy

Khalil Azzaoui,¹ Rachid Essehli,¹ El Miloud Mejdoubi,¹ Brahim El Bali,¹ Michal Dusek,² and Karla Fejfarova²

¹Laboratory of Mineral Solid and Analytical Chemistry LMSAC, Department of Chemistry, Faculty of Sciences, Mohamed 1st University, P.O. Box 717, Oujda 60000, Morocco

²Institute of Physics ASCR, v.v.i., Na Slovance 2, 182 21 Prague 8, Czech Republic

Correspondence should be addressed to Brahim El Bali, b.elbali@fso.ump.ma

Received 5 September 2012; Revised 3 October 2012; Accepted 4 October 2012

Academic Editor: Maurizio Peruzzini

Copyright © 2012 Khalil Azzaoui et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Two new dodecahydrate trisodium triphosphates $\text{Na}_3\text{MP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$ ($\text{M} = \text{Co}$ (1), Ni (2)) were synthesized using a wet chemistry route and characterized by X-ray diffraction and FT-IR spectroscopy. They are isotypic, monoclinic ($\text{P}2_1/n$, $Z = 2$), with pseudoorthorhombic unit cell parameters ($\text{\AA},^\circ$): ($a = 14,9906$ (4), $b = 9,1628$ (2), $c = 14,6660$ (4), $\beta = 90,098$ (2), for (1) and $a = 15,0236$ (3), $b = 9,1972$ (2), $c = 14,6654$ (3), $\beta = 90,0492$ (16) for (2)). Values of R/R_w are 0.0267/0.0738 and 0.0284/0.0907, respectively, for (1) and (2). Both compounds were found to be systematically twinned by 180° rotation around a . Their frameworks are made by slabs parallel to ab plane, resulting from the cohesion of two kinds of metallic chains. IR spectrum confirms the presence of characteristic bands from P_3O_{10} phosphate group.

1. Introduction

Phosphates containing polyanions $\text{P}_n\text{O}_{3n+1}^{(n+2)-}$ ($n = 1$ and 2) have been intensively investigated during the last few decades because of their applications in different fields: solid electrolytes for energy stockage, Li-ion batteries, ceramics, luminescence, and magnetism [1]. Kanonerovite, $\text{Na}_3\text{MnP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$, is a natural triphosphate mineral [2]; few other synthetic triphosphates have been reported in the literature: $\text{Na}_3\text{CuP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$ [3], $\text{LiZn}_2\text{P}_3\text{O}_{10} \cdot 8\text{H}_2\text{O}$ [4], $\text{NaZn}_2\text{P}_3\text{O}_{10} \cdot 9\text{H}_2\text{O}$ [5], and $\text{Na}_3\text{CdP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$ [6]. Anhydrous triphosphates have been also studied: $\text{LiFe}_2\text{P}_3\text{O}_{10}$ [7], $\text{LiM}_2\text{P}_3\text{O}_{10}$, $\text{M} = \text{Co}$ and Ni [8, 9], $\text{RbBe}_2\text{P}_3\text{O}_{10}$ [10], $\text{Cs}_2\text{MP}_3\text{O}_{10}$ ($\text{M} = \text{Ga}, \text{Al}, \text{Cr}$) [11]. These latter ternary phosphates, with the frameworks consisting in associated $[\text{PO}_4]$ and $[\text{MO}_6]$, are efficiently used for waste storage hosts [12]. We deal in the present work with the synthesis and structural study of two new hydrated phases: $\text{Na}_3\text{MP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$, $\text{M} = \text{Co}$ (1) and Ni (2).

2. Experimental

2.1. Synthesis. The title compounds $\text{Na}_3\text{M}(\text{P}_3\text{O}_{10}) \cdot 12\text{H}_2\text{O}$ ($\text{M} = \text{Co}$ (1), Ni (2)) were obtained by mixing two solutions made of following reactants, each dissolved in 10 mL distilled water: $\text{Na}_5\text{P}_3\text{O}_{10}$ (0.3219 g) and, respectively, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (0.2378 g) (1) and $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (0.2375 g) (2). The mixtures were stirred for 1 h and then allowed to stand at room temperature. After 2 weeks pink crystals of compound (1) and light green crystals of compound (2) were collected by filtration. The crystals were washed with a water-ethanol (80 : 20 v/v) mixture.

2.2. Single Crystal Study. The X-ray diffraction data for (1) and (2) were collected in a four-circles diffractometer Gemini of Oxford Diffraction (now Agilent Technologies), using graphite monochromatized $\text{CuK}\alpha$ radiation ($\lambda = 1.54184 \text{ \AA}$) collimated by mirrors, detector Atlas. The intensity data were corrected for Lorentz and polarization effects. A numerical

TABLE 1: Crystal data and details of collection and structure refinement for $\text{Na}_3\text{MP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$ M = Co (1) and Ni (2).

Structural data	(1)	(2)
Empirical formula	$\text{Na}_3\text{CoP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$	$\text{Na}_3\text{NiP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$
Formula weight (g/mol)	597	596.8
Temperature (K)	120	120
Wavelength Mo K_α (Å)	1.54184	1.54184
Crystal system, space group	Monoclinic, P21/n	Monoclinic, P21/n
Unit cell dimensions		
<i>a</i> (Å), α (°)	15.0263(3), 90	14.9906(4), 90
<i>b</i> (Å), β (°)	9.1972(2), 90.0492(16)	9.1628(2), 90.098(2)
<i>c</i> (Å), γ (°)	14.6654(3), 90	14.6660(4), 90
Volume (Å ³), <i>Z</i>	2026.76(7), 4	2014.46(9), 4
<i>D</i> _{calc} (Mg/m ³)	1.9559	1.967
Absorption coefficient (mm ⁻¹)	10.499	5.267
<i>F</i> (0 0 0)	1220	1224
Crystal size (mm)	0.3416 * 0.1882 * 0.1274	0.5021 * 0.0801 * 0.0527
Crystal shape, colour	Prism, pink	Needle, colorless
Limiting indices	$-17 \leq h \leq 17, -10 \leq k \leq 10, -17 \leq l \leq 17$	$-16 \leq h \leq 16, -10 \leq k \leq 10, -16 \leq l \leq 16$
Reflections collected	3534	3181
Independent reflections	3456	3107
Diffractometer	Oxford Diffraction Ltd.	Oxford Diffraction Ltd.
Data/restraints/parameters	3534/24/336	3181/24/336
Goodness-of-fit on <i>F</i> ²	1.61	2.11
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0261, <i>wR</i> ₂ = 0.0735	<i>R</i> ₁ = 0.0277, <i>wR</i> ₂ = 0.0904
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0267, <i>wR</i> ₂ = 0.0738	<i>R</i> ₁ = 0.0284, <i>wR</i> ₂ = 0.0907

absorption correction based on the crystal shape was carried out with the program CrysAlis RED [13]. The structures were solved by Superflip program [14] and refined by a full-matrix least-squares technique based on *F*² with Jana2006 [15]. Both compounds were found to be systematically twinned by 180° rotation around *a*. The refined volume fraction of the major twin domain was 0.628(1) for both samples, confirming exactly the same kind of twinning. Only the major twin domain reflections were used in the refinement, using the twinning matrix for different scaling of the fully overlapped reflections. Influence of possible partial overlaps was negligible, without any need to use hklf5 approach. All nonhydrogen atoms were refined with anisotropic displacement parameters. Positions of hydrogen atoms belonging to water molecules were found in the difference Fourier map and refined with a restrain on their distance to the parent oxygen atom. Their isotropic temperature parameters were calculated as $1.2 * U_{eq}$ of the parent oxygen. Table 1 reports the crystallographic data and experimental details about data collection and structure refinements, while selected bond distances are in Table 2. The structural graphics were created using DIAMOND program [16].

Supplementary tables of crystal structures and refinements, notably atomic positions, full list of bond lengths and angles, and anisotropic thermal parameters, have been deposited with the Inorganic Crystal Structure Database, FIZ, Hermann von Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen, Germany; fax: (+49) 7247 808 132; email: crysdata@fiz-karlsruhe.de. CCDC deposition numbers are,

respectively, 884535 for $\text{Na}_3\text{Co}(\text{P}_3\text{O}_{10}) \cdot 12\text{H}_2\text{O}$ and 884536 for $\text{Na}_3\text{Ni}(\text{P}_3\text{O}_{10}) \cdot 12\text{H}_2\text{O}$.

2.3. IR Measurements. The infrared measurements were performed in transmission geometry using an FTIR Biorad spectrometer FTS-40A with dynamic alignment and a spectral resolution of 2 cm⁻¹ in the range 400–4000 cm⁻¹. 0.2 mg sample per 200 mg KBr has been pressed into pellets.

3. Results and Discussions

$\text{Na}_3\text{MP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$ [M = Co (1), Ni (2)] are isostructural, made by slabs parallel to *ab* plane (Figure 1). A slab results from the cohesion of two kinds of metallic chains, C1 and C2 (Figure 2). The chain C1 consists of [Na(2)O₆] octahedra sharing the edge O15–O16 (water molecules) with strongly deformed tetragonal pyramid [Na(3)O₅]. Such dimmers share a corner O5 (oxygen of P2). In the chain C2, [Na(1)O₆] and [MO₆] octahedra share the face O6 (oxygen of P2), O12 (water), and O19 (water), and they are further connected by a corner O11 (water). The details of the connection between the chains C1 and C2 through O–P–O bridges from the P₃O₁₀ phosphate groups are shown in Figure 3. Two parallel sheets are connected by hydrogen bonds, the most pronounced ones are reported in Table 3. The octahedra [MO₆] (M = Co, Ni) are not directly connected in the structures, the shortest Co–Co and Ni–Ni distances are almost the same, respectively, 5.069(6), and 5.068(7) Å.

TABLE 2: Interatomic distances (Å) and angles (°) in $\text{Na}_3\text{MP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$, M = Co, Ni.

(a)						
Co(1)O ₆ in Na ₃ CoP ₃ O ₁₀ · 12H ₂ O						
Co1	O2	O6	O9	O11	O12	O19
O2	<u>2,061(2)</u>	90,35(8)	94,87(8)	91,45(8)	171,96(8)	91,01(8)
O6	90,35(8)	<u>2,141(2)</u>	90,43(8)	177,32(8)	85,90(8)	85,98(8)
O9	94,87(8)	90,43(8)	<u>2,060(2)</u>	91,40(8)	92,27(8)	173,13(8)
O11	91,45(8)	177,32(8)	<u>91,40(8)</u>	<u>2,116(2)</u>	92,07(8)	91,99(8)
O12	171,96(8)	85,90(8)	92,27(8)	92,07(8)	<u>2,098(2)</u>	81,64(8)
O19	91,01(8)	85,98(8)	173,13(8)	91,99(8)	81,64(8)	<u>2,142(2)</u>
⟨d(Co–O)⟩ = 2,103(2)Å, ∠(O; Co; O)> range from 81,64(8) to 177,32(8)°.						
(b)						
P ₃ O ₁₀ in Na ₃ CoP ₃ O ₁₀ · 12H ₂ O						
P1	O1	O2	O3	O4		
O1	<u>1,505(2)</u>	112,1(1)	114,5(1)	107,0(1)		
O2	112,1(1)	<u>1,523(2)</u>	111,7(1)	107,7(1)		
O3	114,5(1)	111,7(1)	<u>1,510(2)</u>	103,0(1)		
O4	107,0(1)	107,7(1)	103,0(1)	<u>1,619(2)</u>		
P2	O4	O5	O6	O7		
O4	<u>1,594(2)</u>	109,1(1)	109,1(1)	100,9(1)		
O5	109,1(1)	<u>1,479(2)</u>	120,0(1)	105,5(1)		
O6	109,1(1)	120,0(1)	<u>1,495(2)</u>	110,5(1)		
O7	100,9(1)	105,5(1)	110,5(1)	<u>1,594(2)</u>		
P3	O7	O8	O9	O10		
O7	<u>1,624(2)</u>	106,5(1)	107,8(1)	102,3(1)		
O8	106,5(1)	<u>1,506(2)</u>	112,2(1)	113,4(1)		
O9	107,8(1)	112,2(1)	<u>1,519(2)</u>	113,8(1)		
O10	102,3(1)	113,4(1)	113,8(1)	<u>1,521(2)</u>		
∠(P1; O4; P2) = 158,3(2)°, ⟨d(P–O _{INT})⟩ = 1.603 Å, ⟨d(P–O _{TER})⟩ = 1.500 Å, ⟨d(P–O _{ALL})⟩ = 1.553 Å. ∠(P2; O7; P3) = 70.9(2)°, ⟨d(P–O _{INT})⟩ = 1.609 Å, ⟨d(P–O _{TER})⟩ = 1.5507 Å, ⟨d(P–O _{ALL})⟩ = 1.5798 Å.						
(c)						
Ni(1)O ₆ in Na ₃ NiP ₃ O ₁₀ · 12H ₂ O						
Ni1	O2	O6	O9	O11	O12	O19
O2	<u>2,046(2)</u>	90,91(9)	93,51(9)	90,12(9)	173,7(1)	91,51(9)
O6	90,91(9)	<u>2,081(2)</u>	91,32(9)	178,45(9)	86,63(9)	86,27(9)
O9	93,51(9)	91,32(9)	<u>2,052(2)</u>	89,76(9)	92,41(1)	174,5(1)
O11	90,12(9)	178,45(9)	89,76(9)	<u>2,067(2)</u>	92,22(9)	92,55(9)
O12	173,7(1)	86,63(9)	92,41(1)	92,22(9)	<u>2,065(3)</u>	82,5(1)
O19	91,51(9)	86,27(9)	174,5(1)	92,55(9)	82,5(1)	<u>2,097(3)</u>
⟨d(Ni–O)⟩ = 2,0615(2) Å, ∠(O; Ni; O)> range from 82,5(1)°–178,45(9)°						
(d)						
P ₃ O ₁₀ in Na ₃ NiP ₃ O ₁₀ · 12H ₂ O						
P1	O1	O2	O3	O4		
O1	<u>1,501(3)</u>	112,5(1)	114,3(1)	106,91(1)		
O2	112,5(1)	<u>1,524(2)</u>	111,7(1)	107,7(1)		
O3	114,3(1)	111,7(1)	<u>1,513(2)</u>	103,0(1)		
O4	106,91(1)	107,7(1)	103,0(1)	<u>1,624(3)</u>		

(d) Continued.

P_3O_{10} in $Na_3NiP_3O_{10} \cdot 12H_2O$				
P2	O4	O5	O6	O7
O4	<u>1,589(3)</u>	109,2(1)	108,9(1)	100,9(1)
O5	109,2(1)	<u>1,480(2)</u>	119,5(1)	106,0(1)
O6	108,9(1)	119,5(1)	<u>1,499(2)</u>	110,7(1)
O7	100,9(1)	106,0(1)	110,7(1)	<u>1,592(3)</u>
P3	O7	O8	O9	O10
O7	<u>1,627(2)</u>	106,0(1)	107,7(1)	102,4(1)
O8	106,0(1)	<u>1,508(2)</u>	112,1(1)	113,2(1)
O9	107,7(1)	112,1(1)	<u>1,520(2)</u>	114,4(1)
O10	102,4(1)	113,2(1)	114,4(1)	<u>1,516(2)</u>

$\angle(P1; O4; P2) = 157.2(2)^\circ$, $\langle d(P-O_{INT}) \rangle = 1.606 \text{ \AA}$, $\langle d(P-O_{TER}) \rangle = 1.5051 \text{ \AA}$, $\langle d(P-O_{ALL}) \rangle = 1.553 \text{ \AA}$.
 $\angle(P2; O7; P3) = 71.3(2)^\circ$, $\langle d(P-O_{INT}) \rangle = 1.6095 \text{ \AA}$, $\langle d(P-O_{TER}) \rangle = 1.551 \text{ \AA}$, $\langle d(P-O_{ALL}) \rangle = 1.5802 \text{ \AA}$.

TABLE 3: Hydrogen bonding parameters ($\text{\AA}$, $^\circ$) for (1) and (2).

(a)				
(1)	D–H	H · · · A	D–A	D–H · · · A
O11–H11A · · · O8 ⁱ	0.82(3)	1.92(3)	2.741(3)	174(3)
O11–H11B · · · O3 ⁱ	0.82(3)	1.90(3)	2.707(3)	169(3)
O12–H12A · · · O2 ⁱ	0.82(3)	1.95(3)	2.763(3)	169(3)
O12–H12B · · · O20 ⁱ	0.823(19)	1.87(2)	2.685(3)	171(3)
O13–H13B · · · O10 ⁱⁱ	0.83(3)	1.95(3)	2.768(3)	172(3)
O14–H14A · · · O1 ⁱⁱ	0.82(2)	1.95(2)	2.757(3)	167(3)
O14–H14B · · · O1	0.83(2)	1.92(2)	2.735(3)	169(4)
O17–H17A · · · O3 ⁱ	0.82(3)	1.95(3)	2.756(3)	171(3)
O17–H17B · · · O1 ⁱⁱⁱ	0.82(3)	1.87(3)	2.691(3)	174(4)
O19–H19A · · · O9 ⁱ	0.82(2)	1.96(2)	2.773(3)	171(4)
O19–H19B · · · O14 ^{iv}	0.820(19)	1.91(2)	2.728(3)	174(3)
O20–H20B · · · O10 ^v	0.822(14)	1.893(14)	2.712(3)	174(4)
(i) $-x + 1/2, y - 1/2, -z + 1/2$; (ii) $x + 1/2, -y + 1/2, z + 1/2$; (iii) $-x + 1/2, y + 1/2, -z - 1/2$; (iv) $-x + 1/2, y - 1/2, -z + 3/2$; (v) $-x + 1/2, y + 1/2, -z + 1/2$.				
(b)				
(2)	D–H	H · · · A	D–A	D–H · · · A
O11–H11A · · · O8	0.82(3)	1.91(3)	2.736(3)	176(3)
O12–H12A · · · O2	0.82(3)	1.88(3)	2.760(3)	173(4)
O12–H12B · · · O20	0.82(2)	1.88(3)	2.694(4)	173(4)
O16–H16A · · · O18	0.821(16)	1.965(18)	2.784(4)	175(4)
O18–H18A · · · O21 ⁱ	0.82(3)	1.93(3)	2.748(4)	170(3)
O18–H18B · · · O10 ⁱⁱ	0.82(3)	1.96(3)	2.775(3)	177(4)
O19–H19A · · · O9 ⁱⁱⁱ	0.82(3)	1.96(3)	2.775(3)	171(4)
O19–H19B · · · O14	0.82(2)	1.92(3)	2.735(4)	174(4)
O22–H22B · · · O13 ^{iv}	0.82(3)	2.01(3)	2.835(4)	180(4)
(i) $-x + 1/2, y - 1/2, -z + 3/2$; (ii) $x, y, 1 + z$; (iii) $x, y, z - 1$; (iv) $1 - x, -y, 1 - z$.				

Phosphorous (P^{VI}) atoms occupy three symmetrically independent tetrahedrally coordinated positions. The $[PO_4]$ share an apex to build up the triphosphate polyanion P_3O_{10} . Average distances P–O in $P(1)O_4$, $P(2)O_4$, and $P(3)O_4$ are, respectively, 1.5292, 1.5404, and 1.5423 $\text{\AA}$ (see

Table 2 for details), which are of the same magnitude as the values reported in $Na_3Cu(P_3O_{10}) \cdot 12H_2O$ [3] and $Na_3Cd(P_3O_{10}) \cdot 12H_2O$ [6]. P_3O_{10} could be viewed as a combination of two P_2O_7 groups, characterized by the P–O–P angle 133.61(14) and 132.02(13) in (1) and 129.08(14) and

TABLE 4: I-R band assignments for (1) and (2).

Frequency ν (cm ⁻¹)	Assigned vibration mode
3455	ν O–H
1648	ν_s H–OH
1241	ν_{as} PO ₂
1204	ν_{as} PO ₂
1090	ν_s PO ₂
986	ν_s PO ₃
910	ν_{as} POP
690	ν POP
526	δ PO ₃

FIGURE 1: Projection of the crystal structures of $\text{Na}_3\text{MP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$ along b , here the case of (2).

131.36(15) in (2), which is also comparable with the already mentioned known phases. The phosphate group P_3O_{10} acts differently towards metals, being, respectively, monodentate and tridentate with respect to the coordination of Na and M.

The Infrared spectra of (1) and (2) are almost identical, they were recorded in the spectral zone 4000–400 cm⁻¹. Figure 4 depicts the spectrum from the Co phase. Its interpretation can be made on the basis of characteristic vibrations of PO₃ group, POP bridge, and H₂O molecules. Band assignments (Table 4) have been obtained by comparing the results of data reported for known compounds [1]. The asymmetric and symmetric terminal stretching vibrations of the PO₃ groups usually occur in the region 1250–975 cm⁻¹. The bands observed at 1138.75 and 1113.68 cm⁻¹ and 1168.84 cm⁻¹ are assigned to the asymmetric terminal stretching vibration of the PO₃ group $\nu_{as}(\text{PO}_3)$.

The POP bridge vibrations always occur at lower frequency than the terminal P–O stretching modes. In the IR spectra, the asymmetric mode $\nu_{as}(\text{POP})$ gives rise to a band at 872.63 cm⁻¹. Symmetric bridge vibrations $\nu_s(\text{POP})$ appear

FIGURE 2: A slab in the crystal structures of the title compounds.

FIGURE 3: Details of the connection between the chains C1 and C2 inside a slab.

FIGURE 4: IR spectrum of $\text{Na}_3\text{CoP}_3\text{O}_{10} \cdot 12\text{H}_2\text{O}$.

in the IR spectra at 767.52 cm^{-1} . The broad bands in the region ($3450\text{--}3000\text{ cm}^{-1}$) are assigned to the stretching of water molecules $\nu(\text{H}_2\text{O})$. The bands appearing in the spectral region $2900\text{--}2000\text{ cm}^{-1}$ are assigned to the O–H vibrations. Several other weak and medium intensity bands are due to the presence of multiple hydrogen bonds and the field correlation effect. The doublet near 1630 cm^{-1} corresponds to the bending of water molecules $\delta(\text{H}_2\text{O})$.

4. Conclusion

Crystals of the title compounds have been synthesized using a wet chemistry route. $\text{Na}_3\text{MP}_3\text{O}_{10}\cdot 12\text{H}_2\text{O}$ ($\text{M} = \text{Co}, \text{Ni}$) are isostructural and their framework can be described as two kinds of chains connected through O–P–O of P_3O_{10} phosphate groups into slabs parallel with *ab*. The slabs are connected only by hydrogen bonds. IR spectra of the two compounds reveal typical P_3O_{10} bands known for phosphates.

Acknowledgment

The authors would like to thank the Grant Agency of the Czech Republic, Grant P204/11/0809.

References

- [1] D. E. C. Corbridge, Ed., *Phosphorus*, Elsevier, Amsterdam, The Netherlands, 1990.
- [2] V. I. Popova, V. A. Popov, E. V. Sokolova, G. Ferraris, and N. V. Chukanov, "Kanonerovite, $\text{MnNa}_3\text{P}_3\text{O}_{10}\cdot 12\text{H}_2\text{O}$, first triphosphate mineral," *Neues Jahrbuch für Mineralogie, Monatshefte*, no. 3, pp. 117–127, 2002.
- [3] O. Jouini, M. Dabbabi, M. T. Averbuch-Pouchot, A. Durif, and J. C. Guitel, "Structure du triphosphate de cuivre(II) et de trisodium dodécahydraté, $\text{CuNa}_3\text{P}_3\text{O}_{10}\cdot 12\text{H}_2\text{O}$," *Acta Crystallographica*, vol. C40, pp. 728–730, 1984.
- [4] A. S. Lyakhov, V. A. Lyutsko, L. I. Prodan, and K. K. Palkina, "Crystal structure of Lithium Zinc Triphosphate Octahydrate $\text{LiZn}_2\text{P}_3\text{O}_{10}\cdot 8\text{H}_2\text{O}$," *Inorganic Materials*, vol. 27, no. 5, pp. 845–849, 1991.
- [5] M. T. Averbuch-Pouchot and J. C. Guitel, "Structure cristalline du tripolyphosphate mixte zinc-sodium nonahydraté: $\text{Zn}_2\text{NaP}_3\text{O}_{10}\cdot 9\text{H}_2\text{O}$," *Acta Crystallographica*, vol. B33, pp. 1427–1431, 1977.
- [6] V. Lutsko and G. Johansson, "The Crystal structure of trisodium cadmium triphosphate $\text{Na}_3\text{CdP}_3\text{O}_{10}[\text{H}_2\text{O}]_{12}$," *Acta Chemica Scandinavica*, vol. A38, no. 5, pp. 415–417, 1984.
- [7] M. Kopeck, C. V. Ramana, X. Zhang et al., "Synthesis, characterization and electrochemical properties of a novel triphosphate $\text{LiFe}_2\text{P}_3\text{O}_{10}$," *Electrochimica Acta*, vol. 54, no. 23, pp. 5500–5508, 2009.
- [8] F. Breach, A. Boukhari, and E. M. Holt, "Lithium dicobalt tripolyphosphate and lithium dinickel tripolyphosphate," *Acta Crystallographica Section C*, vol. 52, no. 8, pp. 1867–1869, 1996.
- [9] K. Rissouli, K. Benkhoulja, A. Sadel et al., "A new type of triphosphate group: crystal structure and magnetic properties of $\text{Co}_2\text{LiP}_3\text{O}_{10}$," *European Journal of Solid State and Inorganic Chemistry*, vol. 34, pp. 221–230, 1997.
- [10] M.-T. Averbuch-Pouchot and A. Durif, "Synthese et structure cristalline du dihydrogenodiphosphate de caesium," *Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences*, vol. 316, no. 2, pp. 609–617, 1993.
- [11] A. Guesdon, E. Daguts, and B. Raveau, "A series of cesium triphosphates with a layer structure: $\text{Cs}_2\text{MP}_3\text{O}_{10}$ ($\text{M} = \text{Ga}, \text{Al}, \text{Cr}$)," *Journal of Solid State Chemistry*, vol. 167, no. 1, pp. 258–264, 2002.
- [12] E. H. Oelkers and J. M. Montel, "Phosphates and nuclear waste storage," *Elements*, vol. 4, no. 2, pp. 113–116, 2008.
- [13] Agilent, *Crysalis PRO*, Agilent Technologies, Yarnton, UK, 2010.
- [14] L. Palatinus and G. Chapuis, "Superflip—a computer program for the solution of crystal structures by charge flipping in arbitrary dimensions," *Journal of Applied Crystallography*, vol. 40, no. 4, pp. 786–790, 2007.
- [15] V. Petříček, M. Dušek, and L. Palatinus, *Structure Determination Software Programs*, Institute of Physics, Praha, Czech Republic, 2007.
- [16] K. Brandenburg and H. Putz, *Diamond Version 3*, Crystal Impact GbR, Bonn, Germany, 2005.