Electronic Supplementary Material (ESI) for CrystEngComm.

Oxyanion clusters with antielectrostatic hydrogen bonding (AEHB) in tetraalkylammonium hypodiphosphates †

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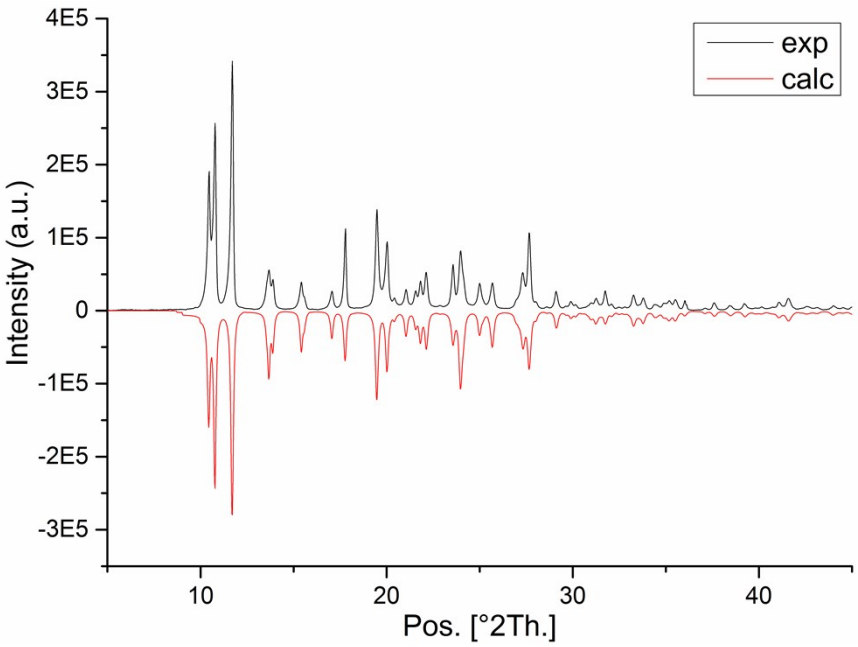
Content:



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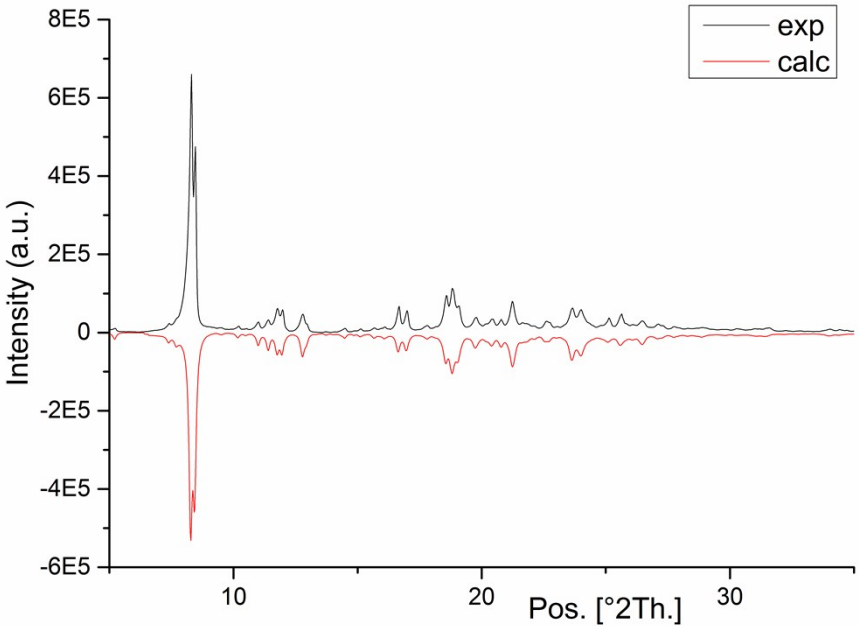

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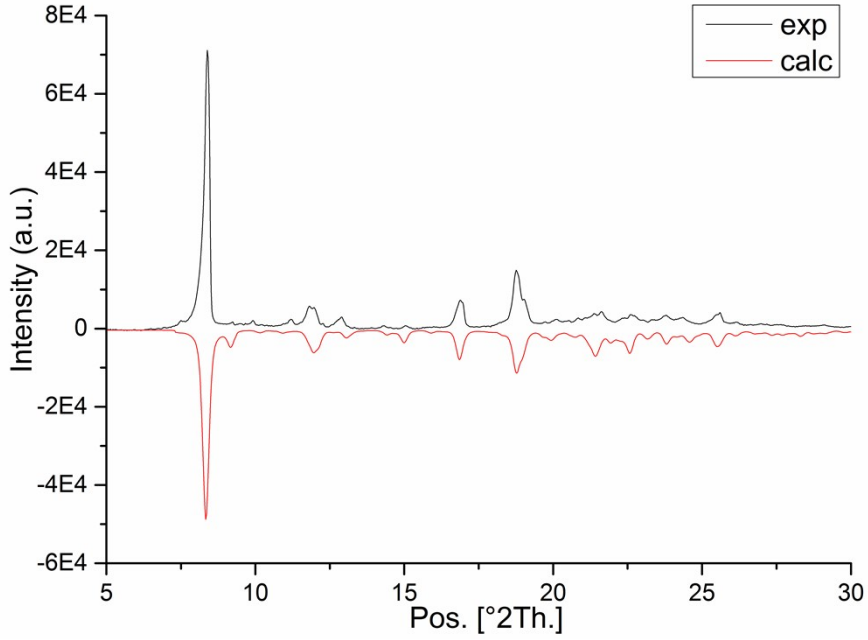
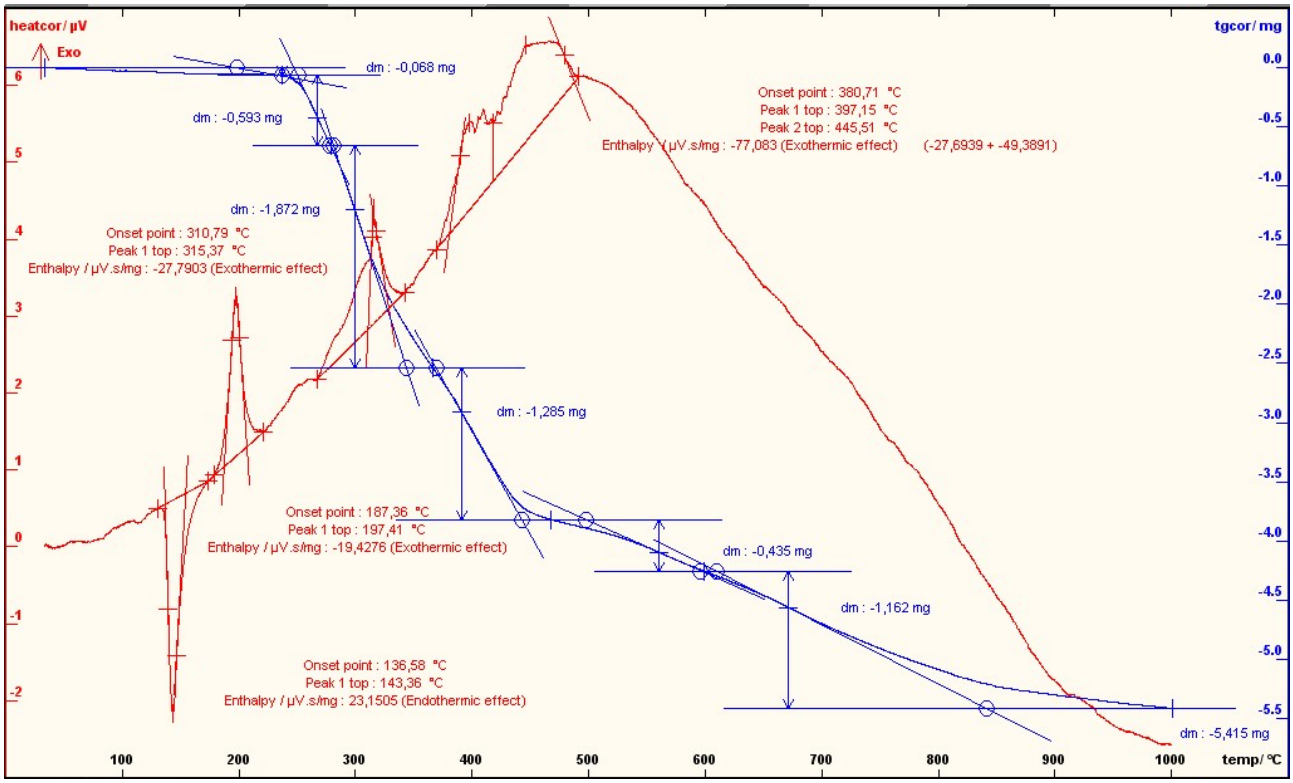
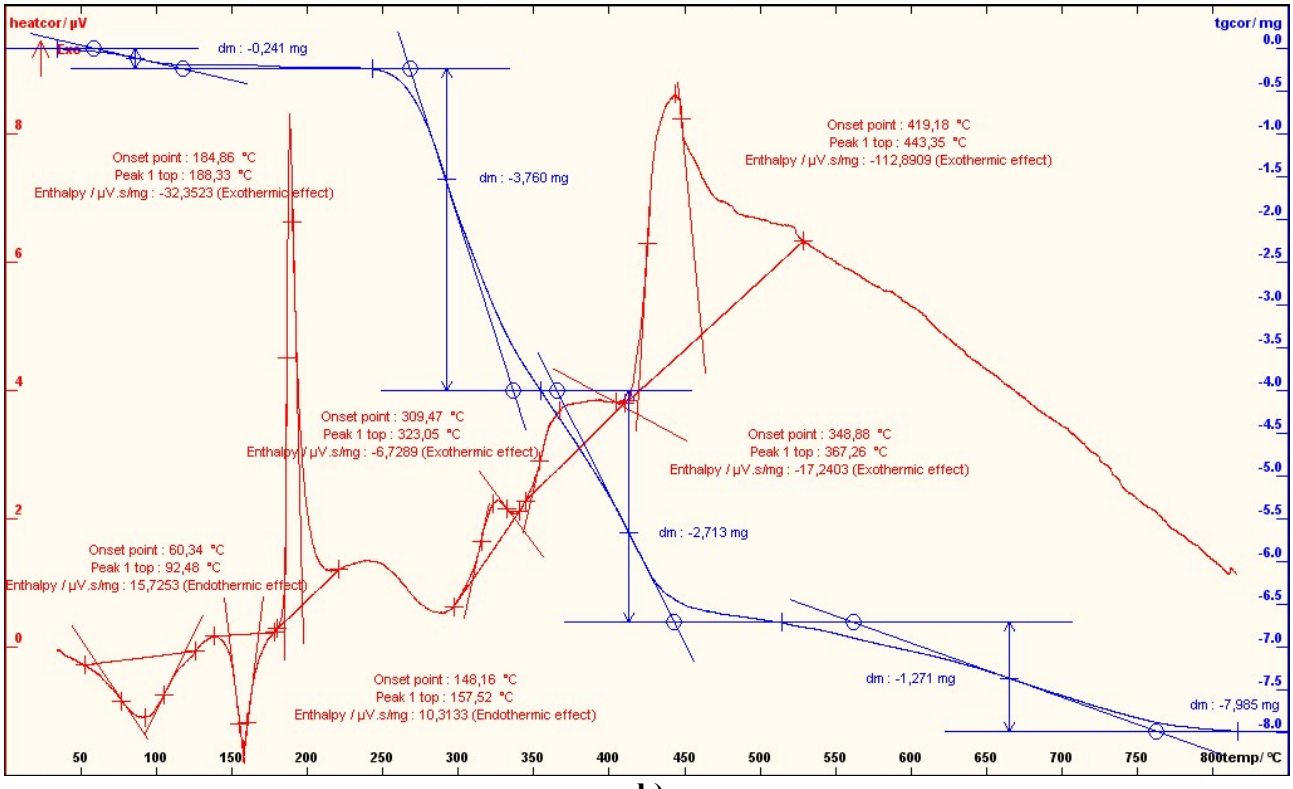


c)

Figure S1. Experimental and calculated powder diffraction patterns for (a)**2**, (b)**4** and (c)**5**.



a)



b)

Figure S2. TG/DTA curves (blue and red, respectively) of **2** and **4**.

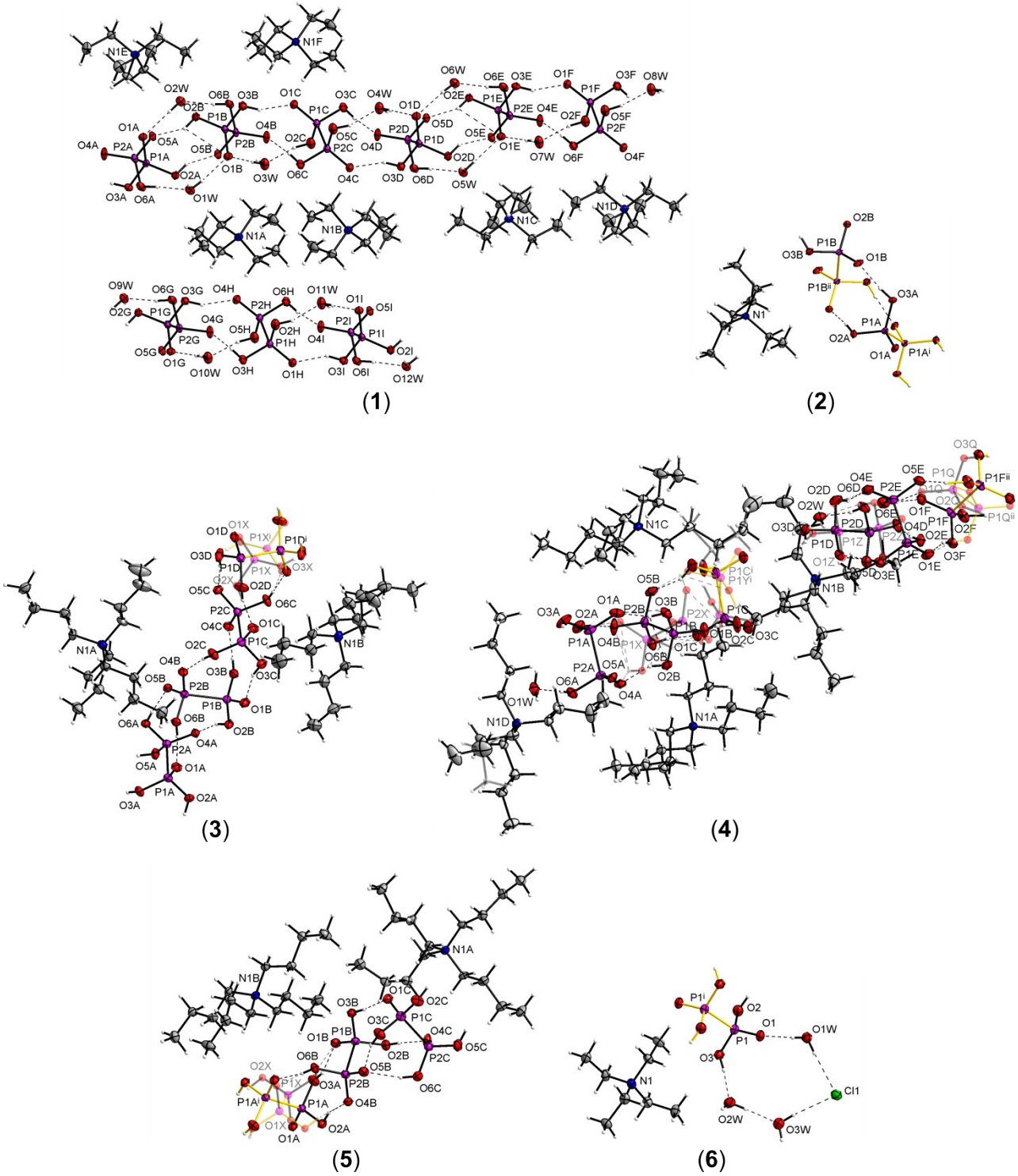


Figure S3. Asymmetric units of **1–6** (black bonds), showing the atom-numbering schemes (for P, O and N atoms) and symmetry–independent hydrogen bonds (dashed lines). Displacement ellipsoids are shown at the 50% probability level. Two positions of the disordered hypodiphosphates in **3** and **4** are shown: with higher occupancy factors – black bonds and labels; with lower SOFs (refined isotropically) – transparent bonds and atoms (shown as spheres) and grey labels. Symmetry codes for **2**, **3**, **4**, **5** and **6** are given in Tables S2-S6.

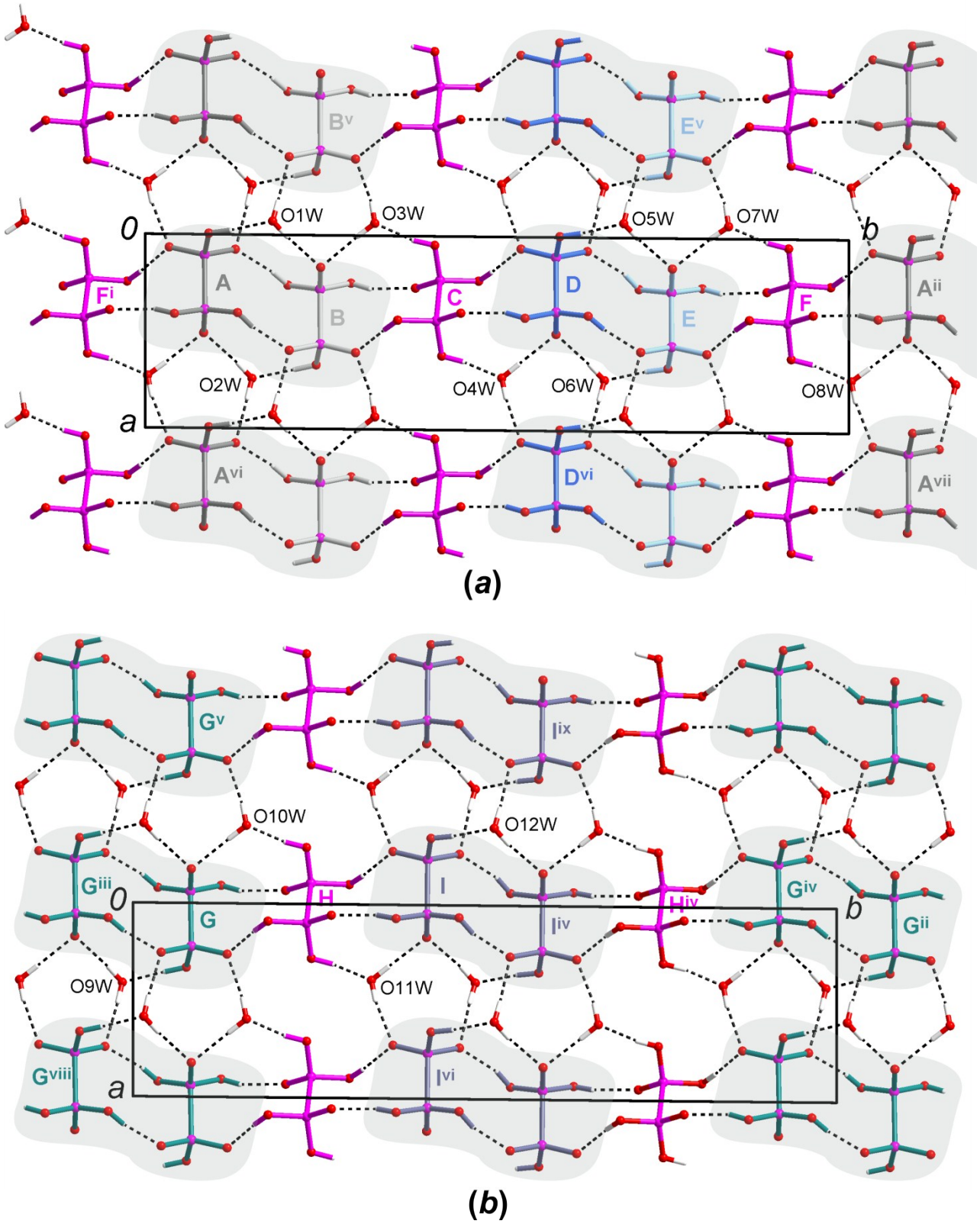


Figure S4. Two different $H_3P_2O_6^-/H_4P_2O_6$ layers in **1**. Crystallographically independent anions are drawn in different colours. Molecules of hypodiphosphoric acid are marked in pink. Hydrogen bonds shown as dashed lines. Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, *y*+1, *z*; (iii) −*x*, −*y*, −*z*+1; (iv) −*x*, −*y*+1, −*z*+1; (v) *x*−1, *y*, *z*; (vi) *x*+1, *y*, *z*; (vii) *x*+1, *y*+1, *z*; (viii) −*x*+1, −*y*, −*z*+1; (ix) −*x*−1, −*y*+1, −*z*+1.AEHB dimers are shadowed with grey background.

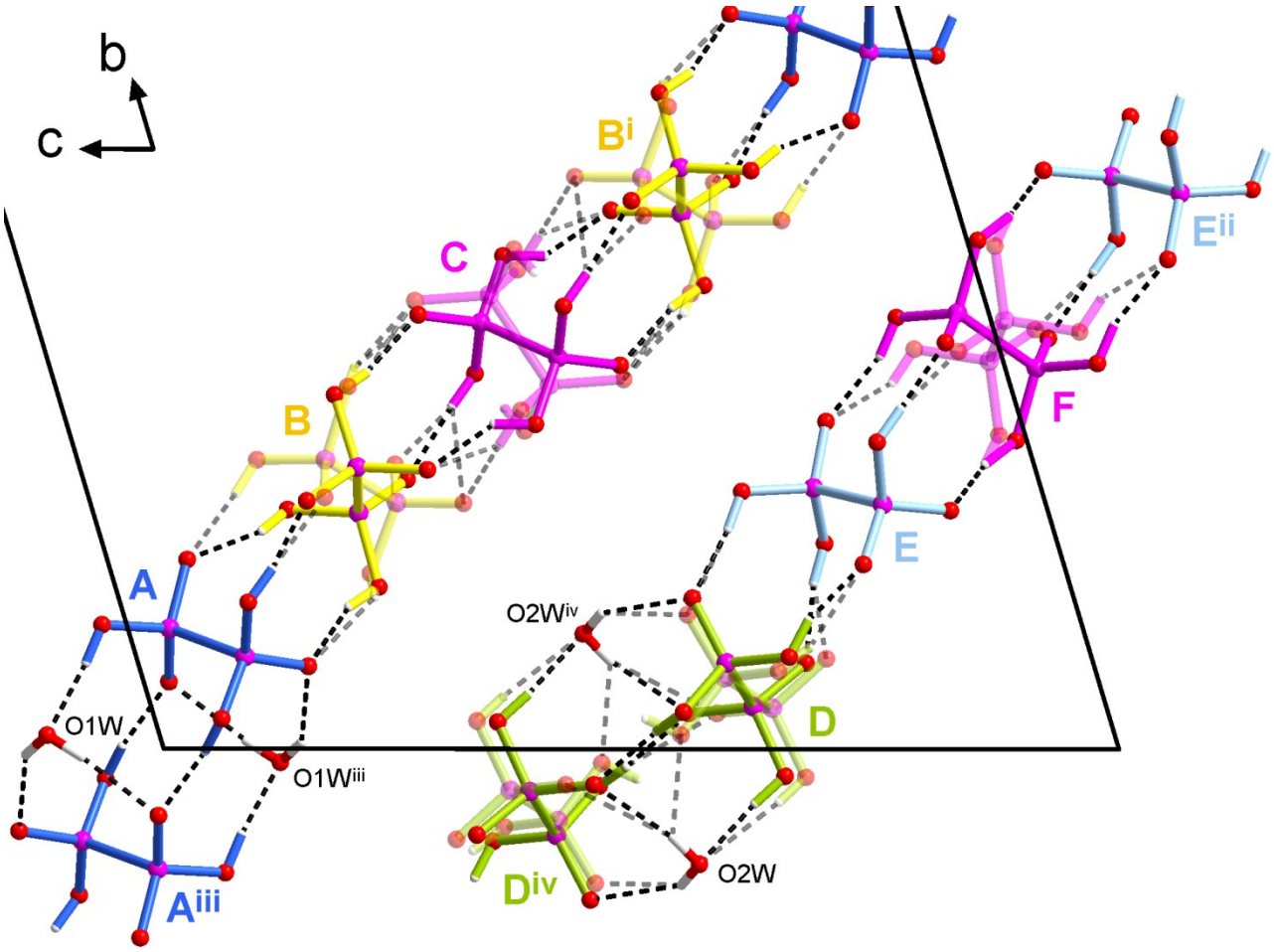


Figure S5. Two different chains in **4** formed by $H_3P_2O_6^-$ (**4-A**,**B**,**D,E**)monoanions, and $H_4P_2O_6$ (**4-C**,**F**; pink) molecules linked by O–H···O hydrogen bonds (dashed lines). Disorder of anions and acid molecules is shown: with higher occupancy factors – thick bonds and black labels; with lower SOFs (refined isotropically) – transparent bonds and atoms and grey label. Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*; (iii) −*x*+1, −*y*, −*z*+2; (iv) −*x*, −*y*, −*z*+1.

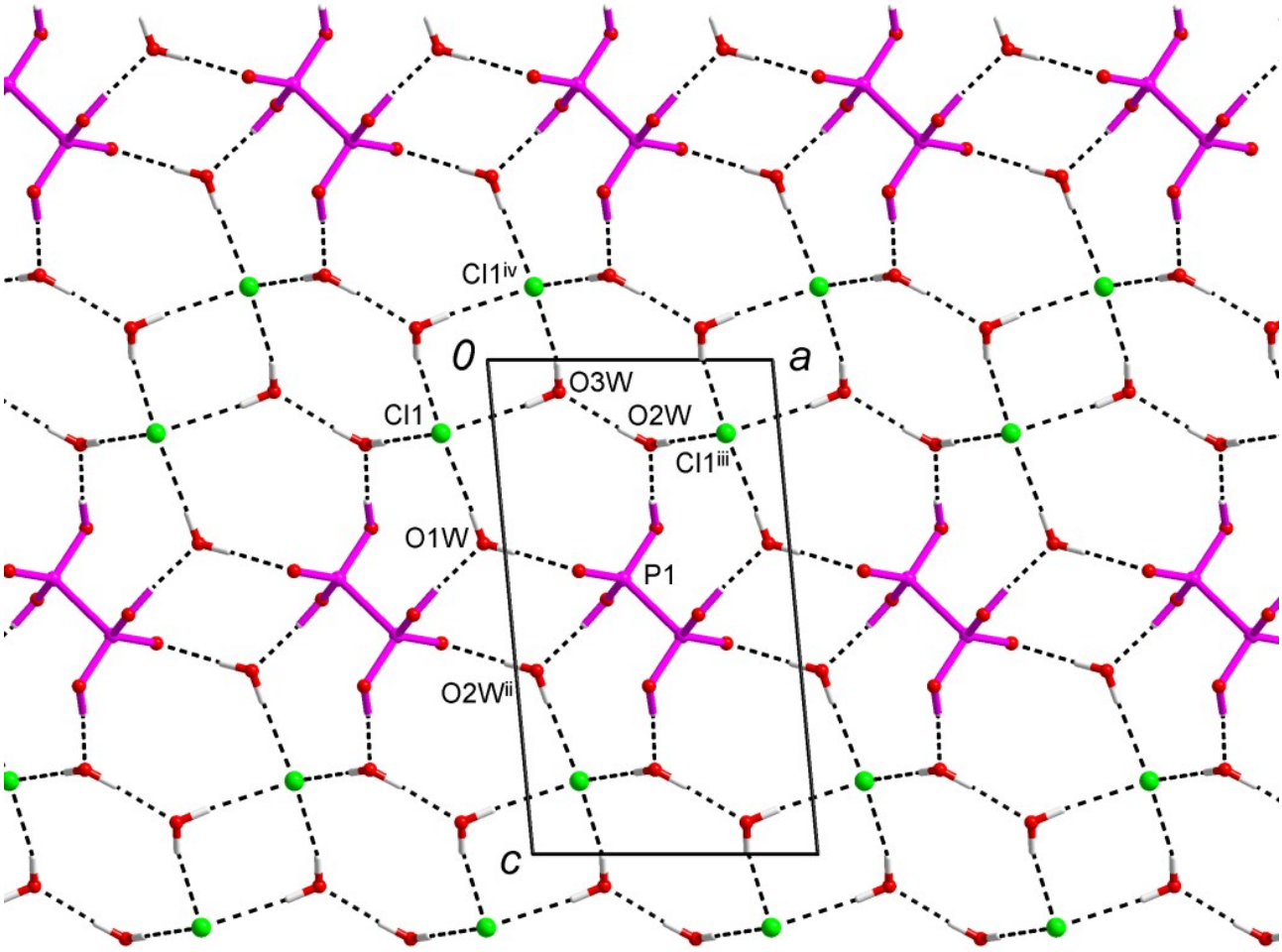


Figure S6. Chains of hydrogen-bonded (dashed lines) $H_4P_2O_6/H_2O$ molecules running down the *a* axis in **6** joined with each other by O–H···O and O–H···Cl hydrogen bonds giving rise to layers parallel to (011) plane. Symmetry codes: (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*, −*y*+2, −*z*.

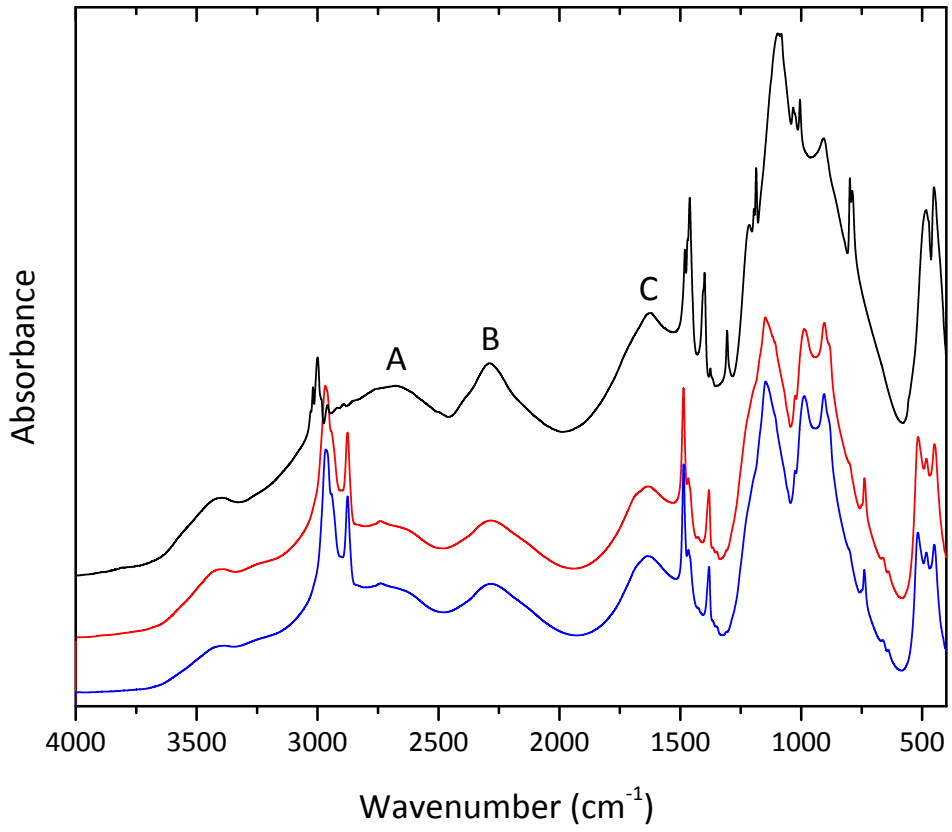


Figure S7. The IR spectra of the compounds **2** (black), **4** (red) and **5** (blue).The letters A, B and C denote the appearance of the structure characteristic for strong hydrogen bonds.

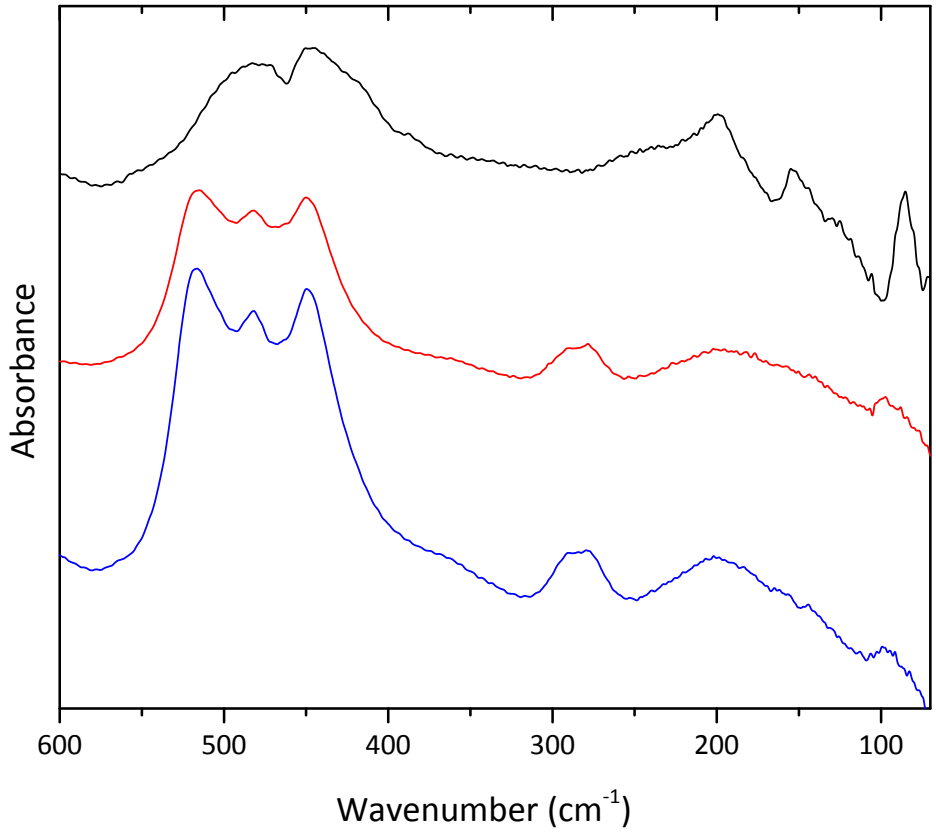


Figure S8. The far IR spectra of the compounds **2** (black), **4** (red) and **5** (blue).

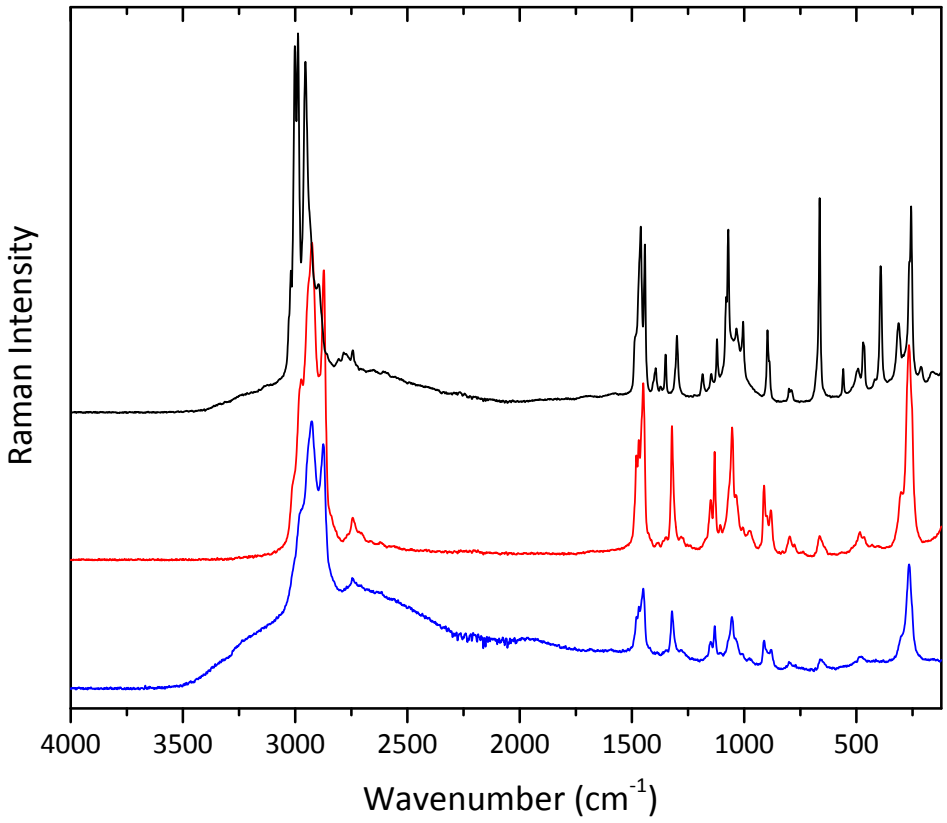


Figure S9. The Raman spectra of the compounds **2** (black), **4** (red) and **5** (blue).

Table S1. Selected geometric parameters (Å, º) for $[(Et_4N)(H_3P_2O_6)]\cdot 0.5H_4P_2O_6\cdot 2H_2O$(**1**). $H_4P_2O_6$ molecules are marked in pink.

	1-A ($H_3P_2O_6^-$)	**1-B** ($H_3P_2O_6^-$)	**1-C** ($H_4P_2O_6$)	**1-D** ($H_3P_2O_6^-$)	**1-E** ($H_3P_2O_6^-$)	**1-F** ($H_4P_2O_6$)	**1-G** ($H_3P_2O_6^-$)	**1-H** ($H_4P_2O_6$)	**1-I** ($H_3P_2O_6^-$)
P1–P2	2.1812(8)	2.1824(8)	2.1791(8)	2.1817(8)	2.1817(8)	2.1797(8)	2.1832(8)	2.1791(8)	2.1796(8)
P1–O1	1.4928(11)	1.4949(11)	1.4912(11)	1.4956(11)	1.4927(11)	1.4920(11)	1.4946(11)	1.4890(11)	1.4918(11)
P1–O2	1.5490(11)	1.5439(11)	1.5464(12)	1.5457(11)	1.5478(11)	1.5470(12)	1.5456(11)	1.5470(12)	1.5475(11)
P1–O3	1.5505(12)	1.5508(12)	1.5586(12)	1.5497(12)	1.5489(11)	1.5582(12)	1.5506(12)	1.5586(12)	1.5478(11)
P2–O4	1.5045(11)	1.5072(11)	1.4897(11)	1.5060(11)	1.5057(11)	1.4921(11)	1.5049(11)	1.4891(11)	1.5061(11)
P2–O5	1.5122(11)	1.5159(12)	1.5477(12)	1.5131(12)	1.5108(11)	1.5491(12)	1.5128(12)	1.5482(12)	1.5140(11)
P2–O6	1.5648(11)	1.5678(11)	1.5571(12)	1.5678(11)	1.5667(11)	1.5551(12)	1.5648(11)	1.5570(12)	1.5654(11)
O1–P1–O2	115.98(6)	116.32(6)	115.85(7)	116.39(6)	116.07(6)	115.48(7)	115.88(6)	115.74(7)	116.32(6)
O1–P1–O3	114.95(6)	114.70(7)	111.59(7)	114.60(7)	115.02(7)	111.79(7)	114.57(7)	111.64(6)	115.10(7)
O2–P1–O3	103.27(6)	103.28(7)	106.84(7)	103.22(7)	103.17(6)	107.05(7)	103.32(6)	107.02(7)	103.16(6)
O1–P1–P2	110.96(5)	109.93(5)	109.42(5)	110.02(5)	110.97(5)	109.50(5)	110.30(5)	109.63(5)	110.68(5)
O2–P1–P2	104.57(5)	104.50(5)	106.85(6)	104.46(5)	104.55(5)	106.87(6)	105.02(5)	106.95(5)	104.17(5)
O3–P1–P2	106.09(5)	107.23(5)	105.72(5)	107.27(5)	106.00(5)	105.58(5)	106.90(5)	105.25(5)	106.33(5)
O4–P2–O5	116.48(7)	116.51(7)	115.86(7)	116.61(7)	116.43(7)	115.48(7)	116.53(7)	115.67(7)	116.55(7)
O4–P2–O6	108.23(7)	108.33(7)	111.56(7)	108.28(7)	108.26(7)	111.74(7)	108.15(7)	111.73(7)	108.32(7)
O5–P2–O6	110.58(6)	110.16(6)	106.92(7)	110.21(6)	110.63(6)	107.13(7)	110.52(6)	106.74(7)	110.16(6)
O4–P2–P1	107.79(5)	108.10(5)	109.39(5)	108.16(5)	107.84(5)	109.58(5)	107.78(5)	109.46(5)	108.04(5)
O5–P2–P1	107.42(5)	107.04(5)	106.86(6)	106.93(5)	107.38(5)	106.83(5)	107.08(5)	106.71(5)	107.40(5)
O6–P2–P1	105.79(5)	106.21(5)	105.68(6)	106.14(5)	105.74(5)	105.51(5)	106.28(5)	105.98(5)	105.83(5)
O1–P1–P2–O4	68.58(7)	−69.28(7)	−179.79(5)	69.29(7)	−68.43(7)	179.80(5)	−70.25(7)	−179.00(5)	68.17(7)
O2–P1–P2–O4	−165.68(7)	165.21(7)	−53.65(7)	−165.08(7)	165.72(7)	−54.45(7)	164.22(7)	54.79(7)	−166.09(7)
O3–P1–P2–O4	−56.91(7)	56.02(7)	59.91(7)	−55.97(7)	57.09(7)	59.29(7)	54.89(7)	−58.80(7)	−57.51(7)
O1–P1–P2–O5	−57.69(7)	56.97(7)	54.06(7)	−57.06(7)	57.77(7)	54.02(7)	55.85(7)	−53.15(7)	−58.33(7)
O2–P1–P2–O5	68.05(6)	−68.55(6)	−179.79(5)	68.57(6)	−68.07(6)	179.78(5)	−69.68(7)	−179.35(5)	67.42(6)
O3–P1–P2–O5	176.83(6)	−177.73(6)	−66.24(7)	177.69(6)	−176.70(6)	−66.48(7)	−179.00(6)	67.05(7)	176.00(6)
O1–P1–P2–O6	−175.83(6)	174.65(6)	−59.57(7)	−174.70(6)	175.93(6)	−59.76(7)	174.00(6)	60.36(7)	−175.99(6)
O2–P1–P2–O6	−50.08(7)	49.13(7)	66.58(7)	−49.07(7)	50.08(6)	65.99(7)	48.47(7)	−65.84(7)	−50.25(7)
O3–P1–P2–O6	58.69(7)	−60.05(7)	−179.87(5)	60.04(7)	−58.55(7)	179.73(5)	−60.85(7)	−179.44(5)	58.33(7)

Table S2. Selected geometric parameters (Å, º) for $[(Et_4N)_2(H_2P_2O_6)]\cdot H_4P_2O_6$ (**2**). $H_4P_2O_6$ molecule is marked in pink.

	2-A ($H_4P_2O_6$)	**2-B** ($H_2P_2O_6^{2-}$)
P1*A*–P1*A*^{i} / P1*B*–P1*B*^{ii}	2.1795(11)	2.1863(12)
P1–O1	1.4931(12)	1.5026(13)
P1–O2	1.5456(12)	1.5169(11)
P1–O3	1.5516(11)	1.5685(12)
O1–P1–O2	111.58(6)	114.75(7)
O1–P1–O3	112.34(7)	108.78(7)
O2–P1–O3	110.69(6)	110.89(6)
O1–P1–P1*A*^{i}/*B*^{ii}	109.42(5)	108.80(6)
O2–P1–P1*A*^{i}/*B*^{ii}	107.66(6)	108.80(6)
O3–P1–P1*A*^{i}/*B*^{ii}	104.82(6)	104.29(6)
O1–P1–P1*A*^{i}/*B*^{ii} –O1*A*^{i}/*B*^{ii}	180	180
O2–P1–P1*A*^{i}/*B*^{ii} –O1*A*^{i}/*B*^{ii}	58.56(7)	−54.34(8)
O3–P1–P1*A*^{i}/*B*^{ii} –O1*A*^{i}/*B*^{ii}	−59.33(7)	64.04(8)
O1–P1–P1*A*^{i}/*B*^{ii} –O2*A*^{i}/*B*^{ii}	−58.56 (7)	54.34(8)
O2–P1–P1*A*^{i}/*B*^{ii} –O2*A*^{i}/*B*^{ii}	180	180
O3–P1–P1*A*^{i}/*B*^{ii} –O2*A*^{i}/*B*^{ii}	62.11(7)	−61.62(7)
O1–P1–P1*A*^{i}/*B*^{ii} –O3*A*^{i}/*B*^{ii}	59.33(7)	−64.04(8)
O2–P1–P1*A*^{i}/*B*^{ii} –O3*A*^{i}/*B*^{ii}	−62.11(7)	61.62(7)
O3–P1–P1*A*^{i}/*B*^{ii} –O3*A*^{i}/*B*^{ii}	180	180

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.

Table S3. Selected geometric parameters (Å, º) for $[(Bu_4N)(H_3P_2O_6)]\cdot 0.75H_4P_2O_6$ (**3**). $H_4P_2O_6$ molecules are marked in pink.

	3-A ($H_4P_2O_6$)	**3-B** ($H_3P_2O_6^-$)	**3-C** ($H_3P_2O_6^-$)	**3-D** ($H_4P_2O_6$) SOF = 0.887(3)
P1–P2 / P1*D*–P1*D*^{i}	2.1722(13)	2.1885(13)	2.1764(13)	2.179(2)
P1–O1	1.478(2)	1.484(2)	1.488(2)	1.480(3)
P1–O2	1.547(2)	1.542(2)	1.531(2)	1.553(4)
P1–O3	1.548(2)	1.560(2)	1.548(2)	1.557(3)
P2–O4	1.498(2)	1.494(2)	1.509(2)	–
P2–O5	1.533(2)	1.519(2)	1.517(2)	–
P2–O6	1.547(2)	1.554(2)	1.557(2)	–
O1–P1–O2	111.90(14)	111.36(13)	112.44(14)	112.7(2)
O1–P1–O3	110.96(13)	113.95(13)	109.49(13)	108.8(3)
O2–P1–O3	110.67(13)	105.95(14)	111.85(14)	111.5(2)
O1–P1–P2/P1*D*^{i}	108.14(10)	109.60(11)	108.71(10)	111.5(2)
O2–P1–P2/P1*D*^{i}	105.46(10)	109.62(10)	108.19(10)	106.6(2)
O3–P1–P2/P1*D*^{i}	109.52(10)	106.15(10)	105.91(11)	105.60(14)
O4–P2–O5	111.56(13)	113.08(13)	114.40(13)	–
O4–P2–O6	115.60(13)	109.57(13)	108.31(13)	–
O5–P2–O6	107.51(13)	111.83(13)	111.64(13)	–
O4–P2–P1	107.58(10)	109.32(10)	109.00(10)	–
O5–P2–P1	109.29(10)	106.98(10)	107.42(10)	–
O6–P2–P1	104.99(10)	105.74(10)	105.68(10)	–
O1–P1–P2/P1*D*^{i}–O4/O1*D*^{i}	64.05(14)	51.66(15)	174.18(14)	180
O2–P1–P2/P1*D*^{i}–O4/O1*D*^{i}	−55.81(14)	174.16(14)	−63.45(14)	56.7(3)
O3–P1–P2/P1*D*^{i}–O4/O1*D*^{i}	−174.93(13)	−71.82(15)	56.61(14)	−62.0(3)
O1–P1–P2/P1*D*^{i}–O5/O2*D*^{i}	−174.66(13)	174.44(13)	−61.36(14)	−56.7(3)
O2–P1–P2/P1*D*^{i}–O5/O2*D*^{i}	65.48(14)	−63.06(14)	61.02(14)	180
O3–P1–P2/P1*D*^{i}–O5/O2*D*^{i}	−53.64(14)	50.95(14)	−178.92(13)	61.3(3)
O1–P1–P2/P1*D*^{i}–O6/O3*D*^{i}	−59.60(14)	−66.22(14)	57.95(14)	62.0(3)
O2–P1–P2/P1*D*^{i}–O6/O3*D*^{i}	−179.45(13)	56.28(15)	−179.67(13)	−61.3(3)
O3–P1–P2/P1*D*^{i}–O6/O3*D*^{i}	61.43(13)	170.30(13)	−59.61(14)	180

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Table S4. Selected geometric parameters (Å, º) for $[(Bu_4N)(H_3P_2O_6)]\cdot 0.25(H_4P_2O_6)\cdot 0.52H_2O$ (**4**). $H_4P_2O_6$ molecules are marked in pink.

	4-A ($H_3P_2O_6^-$)	**4-B** ($H_3P_2O_6^-$) SOF = 0.8680(12)	**4-C** ($H_4P_2O_6$) SOF = 0.8680(12)	**4-D** ($H_3P_2O_6^-$) SOF = 0.897(4)	**4-E** ($H_3P_2O_6^-$)	**4-F** ($H_4P_2O_6$) SOF = 0.9273(18)
P1–P2 / P1*C*–P1*C*^{i} / P1*F*—P1*F*^{ii}	2.1824(9)	2.1795(10)	2.1730(15)	2.1842(12)	2.1812(9)	2.1723(12)
P1–O1	1.4978(17)	1.485(2)	1.499(2)	1.4989(17)	1.4854(16)	1.498(2)
P1–O2	1.5389(17)	1.5423(17)	1.541(2)	1.531(2)	1.5368(16)	1.5145(18)
P1–O3	1.5523(17)	1.565(2)	1.542(2)	1.5475(17)	1.5578(16)	1.5594(16)
P2–O4	1.4946(16)	1.492(3)	–	1.495(2)	1.4947(17)	–
P2–O5	1.5051(15)	1.5149(18)	–	1.5129(17)	1.5212(16)	–
P2–O6	1.5648(16)	1.545(2)	–	1.5670(17)	1.5449(17)	–
O1–P1–O2	114.23(10)	111.62(12)	113.60(13)	114.73(13)	111.20(9)	112.95(12)
O1–P1–O3	113.93(10)	109.84(12)	111.29(17)	114.11(10)	110.38(9)	113.72(12)
O2–P1–O3	103.21(9)	109.34(11)	108.36(16)	102.76(11)	110.30(9)	107.08(12)
O1–P1–P2/P1*C*^{i}/P1*F*^{ii}	106.84(7)	111.22(9)	107.79(12)	106.99(8)	109.51(7)	108.79(11)
O2–P1–P2/P1*C*^{i}/P1*F*^{ii}	108.55(7)	107.81(8)	107.17(11)	108.14(9)	107.48(7)	108.18(9)
O3–P1–P2/P1*C*^{i}/P1*F*^{ii}	109.99(7)	106.86(9)	108.44(11)	109.96(9)	107.86(6)	105.75(7)
O4–P2–O5	117.51(9)	114.53(12)	–	117.59(11)	113.35(10)	–
O4–P2–O6	107.64(9)	109.10(14)	–	107.88(12)	109.19(10)	–
O5–P2–O6	111.52(9)	111.68(13)	–	111.46(10)	112.01(9)	–
O4–P2–P1	105.69(6)	109.55(9)	–	106.71(7)	111.10(7)	–
O5–P2–P1	107.00(6)	107.03(8)	–	105.27(8)	105.34(7)	–
O6–P2–P1	106.85(6)	104.42(10)	–	107.36(9)	105.54(7)	–
O1–P1–P2/P1*C*^{i}/P1*F*^{ii}–O4/O1*C*^{i}/O1*F*^{ii}	−70.87(10)	178.64(15)	180	67.75(12)	169.12(10)	180
O2–P1–P2/P1*C*^{i}/P1*F*^{ii}–O4/O1*C*^{i}/O1*F*^{ii}	52.77(10)	55.96(14)	57.37(15)	−56.34(13)	−69.96(10)	−56.96(15)
O3–P1–P2/P1*C*^{i}/P1*F*^{ii}–O4/O1*C*^{i}/O1*F*^{ii}	165.01(10)	−61.48(14)	−59.4(2)	−167.82(11)	48.97(10)	57.48(13)
O1–P1–P2/P1*C*^{i}/P1*F*^{ii}–O5/O2*C*^{i}/O2*F*^{ii}	55.12(10)	−56.64(14)	−57.37(15)	−57.93(11)	−67.77(10)	56.96(15)
O2–P1–P2/P1*C*^{i}/P1*F*^{ii}–O5/O2*C*^{i}/O2*F*^{ii}	178.76(9)	−179.31(10)	180	177.98(11)	53.16(10)	180
O3–P1–P2/P1*C*^{i}/P1*F*^{ii}–O5/O2*C*^{i}/O2*F*^{ii}	−69.00(10)	63.24(11)	63.22(17)	66.50(10)	172.08(9)	−65.56(13)
O1–P1–P2/P1*C*^{i}/P1*F*^{ii}–O6/O3*C*^{i}/O3*F*^{ii}	174.69(9)		59.4(2)	−176.80(11)	50.90(10)	−57.48(13)
O2–P1–P2/P1*C*^{i}/P1*F*^{ii}–O6/O3*C*^{i}/O3*F*^{ii}	−61.68(10)		−63.22(17)	59.11(13)	171.82(9)	65.56(13)
O3–P1–P2/P1*C*^{i}/P1*F*^{ii}–O6/O3*C*^{i}/O3*F*^{ii}	50.56(10)		180	−52.37(11)	−69.26(10)	180

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*.

Table S5. Selected geometric parameters (Å, º) for $[(Bu_4N)(H_3P_2O_6)]\cdot 0.25(H_4P_2O_6)$ (**5**). $H_4P_2O_6$ molecules are marked inpink.

	5-A ($H_4P_2O_6$) SOF =0.963(2)	**5-B** ($H_3P_2O_6^-$)	**5-C** ($H_3P_2O_6^-$)
P1–P2 / P1*A*–P1*A*^{i}	2.1872(12)	2.1847(8)	2.2211(9)
P1–O1	1.4950(17)	1.4916(14)	1.4943(15)
P1–O2	1.5385(15)	1.5420(15)	1.5269(16)
P1–O3	1.551(2)	1.5582(14)	1.5745(16)
P2–O4	–	1.5106(14)	1.5039(15)
P2–O5	–	1.5109(15)	1.5202(16)
P2–O6	–	1.5635(15)	1.5726(17)
O1–P1–O2	111.53(9)	112.28(8)	116.59(9)
O1–P1–O3	110.04(10)	109.85(8)	113.67(9)
O2–P1–O3	111.76(11)	110.26(8)	103.38(9)
O1–P1–P2/P1*A*^{i}	110.40(10)	108.49(6)	107.50(6)
O2–P1–P2/P1*A*^{i}	106.59(7)	108.05(6)	109.18(7)
O3–P1–P2/P1*A*^{i}	106.34(11)	107.78(6)	105.99(7)
O4–P2–O5	–	114.29(8)	115.60(9)
O4–P2–O6	–	112.62(8)	112.57(9)
O5–P2–O6	–	108.21(8)	104.19(9)
O4–P2–P1	–	107.46(6)	107.14(7)
O5–P2–P1	–	109.43(6)	110.46(7)
O6–P2–P1	–	104.32(6)	106.57(7)
O1–P1–P2/P1*A*^{i}–O4/O1*A*^{i}	180	59.43(9)	0.93(9)
O2–P1–P2/P1*A*^{i}–O4/O1*A*^{i}	58.71(11)	−62.53(9)	−126.42(9)
O3–P1–P2/P1*A*^{i}–O4/O1*A*^{i}	−60.65(12)	178.33(8)	122.82(9)
O1–P1–P2/P1*A*^{i}–O5/O2*A*^{i}	−58.71(11)	−175.94(8)	127.63(9)
O2–P1–P2/P1*A*^{i}–O5/O2*A*^{i}	180	62.10(9)	0.29(10)
O3–P1–P2/P1*A*^{i}–O5/O2*A*^{i}	60.63(13)	−57.04(9)	−110.48(9)
O1–P1–P2/P1*A*^{i}–O6/O3*A*^{i}	60.65(12)	−60.34(9)	−119.78(9)
O2–P1–P2/P1*A*^{i}–O6/O3*A*^{i}	−60.63(13)	177.70(8)	112.87(9)
O3–P1–P2/P1*A*^{i}–O6/O3*A*^{i}	180	58.56(8)	2.10(9)

Symmetrycode: (i) −*x*+1, −*y*+1, −*z*+1.

Table S6. Selected geometric parameters (Å, º) for $[(Et_4N)Cl]\cdot 0.5H_4P_2O_6\cdot 3H_2O$ (**6**). $H_4P_2O_6$ molecule is marked in pink.

	($H_4P_2O_6$)
P1–P1^{i}	2.1863(12)
P1–O1	1.4841(16)
P1–O2	1.5512(16)
P1–O3	1.5524(16)
O1–P1–O2	115.27(9)
O1–P1–O3	115.60(9)
O2–P1–O3	103.03(9)
O1–P1–P1^{i}	111.69(7)
O2–P1–P1^{i}	105.67(7)
O3–P1–P1^{i}	104.45(7)
O1–P1–P1^{i}–O1^{i}	180
O2–P1–P1^{i}–O1^{i}	53.94 (10)
O3–P1–P1^{i}–O1^{i}	−54.36 (10)
O1–P1–P1^{i}–O2^{i}	−53.94 (10)
O2–P1–P1^{i}–O2^{i}	180
O3–P1–P1^{i}–O2^{i}	71.69 (9)
O1–P1–P1^{i}–O3^{i}	54.36 (10)
O2–P1–P1^{i}–O3^{i}	−71.69 (9)
O3–P1–P1^{i}–O3^{i}	180

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table S7. Hydrogen-bond geometry (Å, º) for $[(Et_4N)(H_3P_2O_6)]\cdot 0.5H_4P_2O_6\cdot 2H_2O$ (**1**). Interactions within AEHB anion cluster are marked in blue.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*A*—H2*A*···O5*B*	0.84	1.71	2.4869(16)	154
O3*A*—H3*A*···O4*F*^{i}	0.84	1.77	2.5355(16)	151
O6*A*—H6*A*···O1*W*	0.84	1.73	2.5661(17)	174
O2*B*—H2*B*···O5*A*	0.84	1.71	2.4669(16)	150
O3*B*—H3*B*···O1*C*	0.84	1.76	2.5266(16)	151
O6*B*—H6*B*···O2*W*	0.84	1.74	2.5804(16)	174
O2*C*—H2*C*···O3*W*	0.84	1.67	2.4870(17)	163
O3*C*—H3*C*···O4*D*	0.84	1.71	2.5379(17)	168
O5*C*—H5*C*···O4*W*	0.84	1.68	2.4855(17)	160
O6*C*—H6*C*···O4*B*	0.84	1.71	2.5362(17)	169
O2*D*—H2*D*···O5*E*	0.84	1.71	2.4670(16)	150
O3*D*—H3*D*···O4*C*	0.84	1.76	2.5238(16)	151
O6*D*—H6*D*···O5*W*	0.84	1.74	2.5782(16)	174
O2*E*—H2*E*···O5*D*	0.84	1.71	2.4902(16)	154
O3*E*—H3*E*···O1*F*	0.84	1.77	2.5324(16)	150
O6*E*—H6*E*···O6*W*	0.84	1.73	2.5628(17)	174
O2*F*—H2*F*···O7*W*	0.84	1.67	2.4941(17)	166
O3*F*—H3*F*···O4*A*^{ii}	0.84	1.69	2.5186(17)	169
O5*F*—H5*F*···O8*W*	0.84	1.67	2.4921(17)	167
O6*F*—H6*F*···O4*E*	0.84	1.69	2.5198(17)	168
O2*G*—H2*G*···O5*G*^{iii}	0.84	1.70	2.4702(16)	152
O3*G*—H3*G*···O4*H*	0.84	1.76	2.5370(16)	152
O6*G*—H6*G*···O9*W*	0.84	1.74	2.5762(17)	173
O2*H*—H2*H*···O11*W*	0.84	1.68	2.4920(17)	161
O3*H*—H3*H*···O4*G*	0.84	1.69	2.5262(16)	170
O5*H*—H5*H*···O10*W*	0.84	1.67	2.4908(17)	165
O6*H*—H6*H*···O4*I*	0.84	1.71	2.5324(16)	164
O2*I*—H2*I*···O5*I*^{iv}	0.84	1.72	2.4882(16)	152
O3*I*—H3*I*···O1*H*	0.84	1.77	2.5278(16)	149
O6*I*—H6*I*···O12*W*	0.84	1.73	2.5656(17)	174
O1*W*—H1*W*···O5*B*^{v}	0.84	1.93	2.7659(17)	178
O1*W*—H2*W*···O1*B*	0.84	1.92	2.7526(17)	172
O2*W*—H3*W*···O5*A*^{vi}	0.84	1.92	2.7589(17)	177
O2*W*—H4*W*···O1*A*	0.84	1.95	2.7880(16)	175
O3*W*—H5*W*···O1*B*	0.84	1.90	2.7357(17)	177
O3*W*—H6*W*···O4*B*^{v}	0.84	1.91	2.7351(18)	168
O4*W*—H7*W*···O1*D*	0.84	1.89	2.7338(17)	177
O4*W*—H8*W*···O4*D*^{vi}	0.84	1.91	2.7419(17)	172
O5*W*—H9*W*···O5*E*^{v}	0.84	1.92	2.7611(17)	179
O5*W*—H10*W*···O1*E*	0.84	1.95	2.7852(17)	174
O6*W*—H11*W*···O5*D*^{vi}	0.84	1.92	2.7645(18)	179
O6*W*—H12*W*···O1*D*	0.84	1.91	2.7492(17)	173
O7*W*—H13*W*···O1*E*	0.84	1.90	2.7418(17)	176
O7*W*—H14*W*···O4*E*^{v}	0.84	1.92	2.7394(18)	165
O8*W*—H15*W*···O1*A*^{ii}	0.84	1.90	2.7387(17)	176
O8*W*—H16*W*···O4*A*^{vii}	0.84	1.91	2.7401(18)	169
O9*W*—H17*W*···O5*G*^{viii}	0.84	1.93	2.7691(17)	177
O9*W*—H18*W*···O1*G*^{iii}	0.84	1.93	2.7718(17)	175
O10*W*—H19*W*···O4*G*^{v}	0.84	1.91	2.7394(17)	171
O10*W*—H20*W*···O1*G*	0.84	1.90	2.7403(17)	178
O11*W*—H21*W*···O1*I*	0.84	1.90	2.7394(17)	179

O11*W*—H22*W*···O4*I*^{vi}	0.84	1.91	2.7379(17)	167
O12*W*—H23*W*···O5*I*^{ix}	0.84	1.92	2.7561(18)	176
O12*W*—H24*W*···O1*I*^{iv}	0.84	1.92	2.7555(17)	171
C1*A*—H1*A*2···O6*G*	0.99	2.58	3.5107(19)	157
C2*A*—H2*A*3···O1*W*^{vi}	0.98	2.61	3.574(2)	168
C5*A*—H5*A*1···O5*B*	0.99	2.48	3.3820(18)	152
C7*A*—H7*A*1···O2*A*	0.99	2.41	3.3712(18)	164
C8*A*—H8*A*3···O4*H*	0.98	2.54	3.506(2)	167
C3*B*—H3*B*1···O6*D*	0.99	2.52	3.4536(19)	157
C3*B*—H3*B*2···O3*D*^{v}	0.99	2.61	3.284(2)	125
C4*B*—H4*B*1···O12*W*^{ix}	0.98	2.59	3.552(2)	167
C5*B*—H5*B*2···O5*I*	0.99	2.45	3.3496(18)	151
C7*B*—H7*B*1···O2*I*^{iv}	0.99	2.48	3.4367(18)	162
C8*B*—H8*B*1···O4*C*	0.98	2.57	3.538(2)	168
C1*C*—H1*C*1···O6*I*^{iv}	0.99	2.40	3.246(2)	143
C1*C*—H1*C*2···O1*H*^{iv}	0.99	2.42	3.3556(19)	158
C2*C*—H2*C*1···O5*W*	0.98	2.58	3.542(2)	166
C7*C*—H7*C*1···O1*E*	0.99	2.61	3.2947(19)	127
C3*D*—H3*D*1···O4*F*	0.99	2.39	3.3368(19)	161
C3*D*—H3*D*2···O6*A*^{ii}	0.99	2.45	3.2863(19)	142
C5*D*—H5*D*1···O2*G*^{ii}	0.99	2.54	3.5161(19)	171
C7*D*—H7*D*1···O1*G*^{iv}	0.99	2.61	3.3146(19)	128
C3*E*—H3*E*1···O1*F*^{x}	0.99	2.39	3.3370(19)	160
C3*E*—H3*E*2···O6*E*^{x}	0.99	2.43	3.2715(19)	142
C4*E*—H4*E*3···O2*W*	0.98	2.59	3.554(2)	168
C5*E*—H5*E*2···O2*B*	0.99	2.59	3.5702(19)	171
C7*E*—H7*E*2···O1*A*	0.99	2.61	3.2979(19)	127
C1*F*—H1*F*2···O6*B*	0.99	2.54	3.4751(19)	157
C2*F*—H2*F*3···O6*W*^{xi}	0.98	2.61	3.568(2)	167
C5*F*—H5*F*1···O5*D*^{x}	0.99	2.48	3.3840(18)	151
C7*F*—H7*F*2···O2*E*^{x}	0.99	2.43	3.3867(18)	163
C8*F*—H8*F*3···O1*C*	0.98	2.56	3.522(2)	167

Symmetrycodes: (i) *x*, *y*−1, *z*; (ii) *x*, *y*+1, *z*; (iii) −*x*, −*y*, −*z*+1; (iv) −*x*, −*y*+1, −*z*+1; (v) *x*−1, *y*, *z*; (vi) *x*+1, *y*, *z*; (vii) *x*+1, *y*+1, *z*; (viii) −*x*+1, −*y*, −*z*+1; (ix) −*x*−1, −*y*+1, −*z*+1; (x) −*x*+1, −*y*+1, −*z*; (xi) −*x*+2, −*y*+1, −*z*.

Table S8. Hydrogen-bond geometry (Å, º) for $[(Et_4N)_2(H_2P_2O_6)]\cdot H_4P_2O_6$ (**2**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*A*—H2*A*···O2*B*^{ii}	0.84	1.64	2.4754(18)	173
O3*A*—H3*A*···O1*B*	0.84	1.63	2.4631(15)	172
O3*B*—H3*B*···O1*A*^{iii}	0.84	1.71	2.5483(15)	172
C1—H12···O2*B*^{ii}	0.99	2.45	3.263(2)	140
C3—H32···O1*A*^{iv}	0.99	2.58	3.294(2)	129
C6—H61···O1*A*^{iv}	0.98	2.55	3.527(3)	175
C8—H83···O1*A*^{v}	0.98	2.60	3.571(2)	172

Symmetrycodes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*+1, *z*; (iv) *x*, *y*+1, *z*−1; (v) −*x*, −*y*+1, −*z*+1.

Table S9. Hydrogen-bond geometry (Å, º) for $[(Bu_4N)(H_3P_2O_6)]\cdot 0.75H_4P_2O_6$ (**3**). Interactions within AEHB anion cluster are marked in blue.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*A*—H2*A*···O5*B*^{ii}	0.84	1.74	2.570(3)	168
O3*A*—H3*A*···O4*C*^{ii}	0.84	1.73	2.545(3)	164
O5*A*—H5*A*···O5*C*^{ii}	0.84	1.67	2.511(3)	176
O6*A*—H6*A*···O5*B*	0.84	1.69	2.530(3)	174
O2*B*—H2*B*···O4*A*	0.84	1.72	2.541(3)	164
O3*B*—H3*B*···O4*C*	0.84	1.77	2.606(3)	177
O6*B*—H6*B*···O1*A*	0.84	1.71	2.548(3)	173
O2*C*—H2*C*···O4*B*	0.84	1.63	2.459(3)	169
O3*C*—H3*C*···O1*B*	0.84	1.73	2.540(3)	162
O6*C*—H6*C*···O1*D*^{i}	0.84	1.71	2.552(5)	175
O6*C*—H6*C*···O1*X*^{i}	0.84	1.50	2.33(2)	169
O2*D*—H2*D*···O1*C*	0.84	1.68	2.491(5)	161
O2*X*—H2*X*···O1*C*	0.84	1.68	2.52(3)	175
O3*D*—H3*D*···O5*C*	0.84	1.77	2.603(3)	171
C1*A*—H1*A*2···O3*B*^{iii}	0.99	2.60	3.363(4)	134
C9*A*—H9*A*2···O4*A*^{iv}	0.99	2.47	3.408(4)	158
C1*B*—H1*B*2···O1*C*	0.99	2.34	3.161(4)	140
C5*B*—H5*B*2···O1*D*^{i}	0.99	2.60	3.334(5)	132
C9*B*—H9*B*1···O1*A*^{v}	0.99	2.38	3.271(4)	149

Symmetrycodes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iii) *x*+1, *y*, *z*; (iv) −*x*+3/2, *y*+1/2, −*z*+3/2; (v) −*x*+1, −*y*, −*z*+1.

Table S10. Hydrogen-bond geometry (Å, º) for $[(Bu_4N)(H_3P_2O_6)]\cdot 0.25(H_4P_2O_6)\cdot 0.52H_2O$ (**4**). Interactions within AEHB anion cluster are marked in blue.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*A*—H2*A*···O4*B*	0.84	1.59	2.428(3)	172
O2*A*—H2*A*···O1*X*	0.84	1.86	2.696(10)	178
O3*A*—H3*A*···O5*A*^{iii}	0.84	1.70	2.521(2)	167
O6*A*—H6*A*···O1*W*	0.84	1.75	2.580(2)	171
O2*B*—H2*B*···O4*A*	0.84	1.68	2.469(2)	155
O3*B*—H3*B*···O1*A*	0.84	1.73	2.535(3)	161
O6*B*—H6*B*···O1*C*	0.84	1.68	2.511(4)	167
O2*X*—H2*X*···O4*A*	0.84	1.76	2.480(9)	143
O3*X*—H3*X*···O1*Y*	0.84	1.87	2.502(14)	131
O6*X*—H6*X*···O1*A*	0.84	2.22	2.861(8)	133
O2*C*—H2*C*···O1*B*	0.84	1.73	2.545(3)	162
O3*C*—H3*C*···O5*B*^{i}	0.84	1.70	2.432(3)	145
O3*Y*—H3*Y*···O5*X*^{i}	0.84	1.82	2.572(15)	148
O2*D*—H2*D*···O4*E*	0.84	1.59	2.399(3)	160
O3*D*—H3*D*···O5*D*^{iv}	0.84	1.71	2.494(2)	155
O6*D*—H6*D*···O2*W*	0.84	1.77	2.601(3)	170
O2*Z*—H2*Z*···O4*E*	0.84	2.01	2.754(13)	147
O6*Z*—H6*Z*···O2*W*	0.84	2.16	2.992(16)	169
O2*E*—H2*E*···O4*D*	0.84	1.64	2.461(2)	167
O2*E*—H2*E*···O4*Z*	0.84	1.56	2.345(13)	154
O3*E*—H3*E*···O1*D*	0.84	1.71	2.545(2)	172
O3*E*—H3*E*···O1*Z*	0.84	1.94	2.775(11)	172
O6*E*—H6*E*···O1*F*	0.84	1.67	2.512(3)	178
O6*E*—H6*E*···O1*Q*	0.84	1.67	2.494(16)	168
O2*F*—H2*FE*···O5*E*^{ii}	1.07(3)	1.37(3)	2.420(2)	164(2)
O3*F*—H3*F*···O1*E*	0.84	1.74	2.542(2)	160
O2*Q*—H2*QE*···O5*E*^{ii}	1.23(3)	1.37(3)	2.53(2)	153(2)
O3*Q*—H3*Q*···O1*E*^{ii}	0.84	1.61	2.394(16)	155
O1*W*—H1*W*···O5*A*^{iii}	0.84	1.99	2.775(2)	156
O1*W*—H2*W*···O1*A*^{iii}	0.84	2.03	2.781(2)	149
O2*W*—H3*W*···O5*D*^{iv}	0.84	1.94	2.761(2)	164
O2*W*—H3*W*···O3*Z*	0.84	2.18	2.827(12)	133
O2*W*—H3*W*···O5*Z*^{iv}	0.84	2.58	3.387(12)	163
O2*W*—H4*W*···O1*D*^{iv}	0.84	2.12	2.837(3)	144
O2*W*—H4*W*···O1*Z*^{iv}	0.84	1.86	2.501(14)	132
C1*A*—H1*A*2···O2*B*	0.99	2.51	3.377(3)	146
C2*A*—H2*A*1···O5*E*^{v}	0.99	2.51	3.454(3)	159
C2*A*—H2*A*2···O3*Q*^{v}	0.99	2.48	3.394(19)	154
C5*A*—H5*A*1···O2*B*	0.99	2.56	3.425(3)	146
C9*A*—H9*A*1···O5*E*^{v}	0.99	2.39	3.271(3)	148
C13*A*—H13*A*···O3*F*^{vi}	0.99	2.55	3.509(3)	162
C1*B*—H1*B*2···O2*C*	0.99	2.34	3.284(3)	159
C5*B*—H5*B*1···O6*B*^{i}	0.99	2.50	3.392(3)	149
C5*B*—H5*B*1···O3*X*^{i}	0.99	2.37	3.212(6)	142
C5*B*—H5*B*2···O1*C*^{i}	0.99	2.57	3.210(3)	122
C8*B*—H8*B*3···O1*C*^{i}	0.98	2.57	3.526(5)	164
C9*B*—H9*B*1···O1*D*	0.99	2.50	3.385(3)	148
C10*B*—H10*C*···O3*W*^{i}	0.99	2.58	3.434(15)	144
C15*B*—H15*C*···O1*F*	0.99	2.60	3.322(3)	130
C1*C*—H1*C*1···O3*W*^{i}	0.99	2.47	3.204(15)	131
C1*C*—H1*C*2···O3*B*	0.99	2.43	3.256(3)	140

C5*C*—H5*C*1···O5*B*	0.99	2.36	3.267(3)	151
C9*C*—H9*C*2···O2*D*^{vii}	0.99	2.54	3.368(3)	141
C9*C*—H9*C*2···O2*Z*^{vii}	0.99	2.40	3.275(12)	147
C11*C*—H11*F*···O2*D*^{vii}	0.99	2.42	3.328(3)	153
C1*D*—H1*D*2···O2*F*^{i}	0.99	2.41	3.231(3)	140
C1*D*—H1*D*2···O2*Q*^{i}	0.99	2.22	3.02(2)	137
C5*D*—H5*D*1···O2*E*^{viii}	0.99	2.54	3.511(3)	167
C5*D*—H5*D*2···O3*Q*^{i}	0.99	2.58	3.34(2)	134
C9*D*—H9*D*1···O6*A*	0.99	2.37	3.320(3)	161

Symmetrycodes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*; (iii) −*x*+1, −*y*, −*z*+2; (iv) −*x*, −*y*, −*z*+1; (v) *x*, *y*, *z*+1; (vi) −*x*, −*y*+1, −*z*+1; (vii) −*x*+1, −*y*, −*z*+1; (viii) *x*+1, *y*, *z*+1.

Table S11. Hydrogen-bond geometry (Å, º) for $[(Bu_4N)(H_3P_2O_6)]\cdot 0.25(H_4P_2O_6)$(**5**). Interactions within AEHB anion cluster are marked in blue.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*A*—H2*A*···O4*B*	0.84	1.66	2.456 (2)	157
O3*A*—H3*A*···O1*B*	0.84	1.76	2.539 (3)	153
O2*X*—H2*X*···O4*B*^{i}	0.84	1.74	2.56 (4)	165
O3*X*—H3*X*···O1*B*	0.84	1.66	2.36 (6)	139
O2*B*—H2*B*···O4*C*	0.84	1.66	2.493 (2)	174
O3*B*—H3*B*···O1*C*	0.84	1.71	2.545 (2)	174
O6*B*—H6*B*···O1*A*^{i}	0.84	1.70	2.534 (2)	171
O6*B*—H6*B*···O1*X*^{i}	0.84	1.65	2.49 (4)	173
O2*C*—H2*C*···O5*C*^{ii}	0.84	1.62	2.437 (2)	166
O3*C*—H3*C*···O5*B*	0.84	1.80	2.613 (2)	162
O5*C*—H5*C*···O2*C*^{ii}	0.84	1.62	2.437 (2)	164
O6*C*—H6*C*···O5*B*	0.84	1.81	2.628 (2)	164
C1*A*—H1*AA*···O2*C*^{ii}	0.99	2.60	3.346 (2)	132
C5*A*—H5*AA*···O1*C*	0.99	2.56	3.515 (3)	161
C5*A*—H5*AB*···O5*C*^{ii}	0.99	2.52	3.329 (2)	139
C1*B*—H1*BA*···O1*B*	0.99	2.47	3.308 (2)	143
C1*B*—H1*BB*···O2*X*	0.99	2.45	3.42 (4)	166
C3*B*—H3*BA*···O1*B*	0.99	2.57	3.366 (2)	137
C6*B*—H6*BB*···O2*X*^{iii}	0.99	2.50	3.12 (5)	120
C13*B*—H13*D*···O6*B*^{iv}	0.99	2.49	3.474 (2)	175

Symmetrycodes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+2; (iii) *x*, −*y*+3/2, *z*+1/2; (iv) −*x*+1, *y*+1/2, −*z*+3/2.

Table S12. Hydrogen-bond geometry (Å, º) for $[(Et_4N)Cl]\cdot 0.5H_4P_2O_6\cdot 3H_2O$ (**6**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1*W*^{ii}	0.84	1.69	2.524(2)	176
O3—H3···O2*W*	0.84	1.66	2.488(2)	170
O1*W*—H1*W*···Cl1	0.84	2.31	3.151(2)	178
O1*W*—H2*W*···O1	0.84	1.87	2.710(2)	177
O2*W*—H3*W*···Cl1^{iii}	0.84	2.26	3.0930(19)	172
O2*W*—H4*W*···O3*W*	0.84	1.82	2.659(3)	175
O3*W*—H5*W*···Cl1	0.84	2.31	3.149(2)	174
O3*W*—H6*W*···Cl1^{iv}	0.84	2.35	3.171(2)	167

Symmetrycodes: (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*, −*y*+2, −*z*.

Table S13. The assignment of the bands of compounds **2**, **4** and **5** at room temperature. The abbreviations are explained at the foot of the table.

2		**4**		**5**		**Assignment**
IR	**Raman**	**IR**	**Raman**	**IR**	**Raman**	
3391m		3392m		3387m		νH_2O
3029m						
3019m	3019s		3006sh		2998sh	$\nu_{as}CH_3$
3000m	3001vs	2968m2962sh	2973s	2966m	2967s	$\nu_{as}CH_2$
2984m	2988vs	2944m	2942sh	2960sh	2939sh	νH_2O
2959m			2926vs	2944m	2927vs	
2920w	2955vs					ν_sCH_3
2891w		2876m	2872vs	2876m	2875vs	ν_sCH_2
		2739w	2742vw	2737w	2741vw	overtone
2678m		2688w		2685w		νOH...O (A band)
2289m		2283m		2279m		νOH...O (B band)
1622m		1634m		1634m		νOH...O (C band)
1481m	1487w	1487m	1480m	1486m	1480m	
1470m	1480sh	1466w	1469m	1466w	1469m	$\delta_{as}CH_3$
1461m	1461m	1460sh	1450m	1460sh	1450m	
	1443m					
1405m		1426vw		1424vw		δ_sCH_2
1400m		1382w		1381w		
1376w	1394vw	1365vw		1366vw		
1367vw	1351w	1348vw		1350vw		
1306m	1300w		1322m		1322m	$\omega CH_2\delta OH$
1214s	1186vw	1193sh	1149w	1196sh	1149vw	τCH_2
1194s	1147vw	1149vs	1132w	1148vs	1131w	νH_2O δOH...O
1186s	1122w	1112sh	1106vw	1112sh		νPO
1097vs	1081w		1065sh		1069sh	νCC
1081vs	1071m		1054m		1054m	νCN
1032s	1034w	1024s	1036w	1025s	1036sh	νPO
1027sh						
1005s	1004w	987vs	1005vw	987vs	1004vw	νPO
			973vw		969vw	τH_2O
908s	896w	903s	912w 900w	906s	911w	$\nu PO\rho CH_2$
	888sh	883s	880vw	889sh	880vw	ρCH_3
799s	801vw	802w		804w		νCCN
789s	789vw					
		738m		739m		νCCCN
	664s		664w		656vw	δPO
	559w	517s		517s		
485s	493vw	482s	486w	482s	477vw	δPO
			466vw			
472s 451s	469w	448s		449s		δPO
	392w 312w		302w	300m	297w	δPO
240sh	261sh	291m 278m	266s 254sh	279m	266s 252sh	νPP
	256m					
198m		194m		199m		δPO δCCCN
155w						lattice
85m						

Key: s-very strong, s-strong, m-medium, w-weak, vw-very weak; ν_s–symmetric stretching, ν_{as}-asymmetric stretching, ν_s–symmetric stretching, ν_{as}–asymmetric stretching, δ_{as}-asymmetric bending, δ_s, δ-symmetric bending (scissoring), ρ-rocking, ω-wagging, τ-twisting (torsion), T–translation, L–libration.