Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

FT-IR analyses of compounds were performed using nujol mulls technique with a wavelength between 4000 to 400 cm^{-1}. The recorded spectra are shown in Figures S1–S4. The absorption frequencies around 2925, 1462, 1377 cm^{-1} are derived from nujol. Absorption frequencies 3388–3343 cm^{-1} (N–H stretching), 2725–2706 cm^{-1} (aromatic C–H stretching), 1671-1619 cm^{-1} (N–H in-plane bending), 1600–1300 cm^{-1} (aromatic C=C stretching), 950–700 cm^{-1} (ring breathing), 660–620 cm^{-1} (NH_2 out-of-plane bending) and 560–552 cm^{-1} (C–N–C out-of-plane bending) confirm the 2-aminopyridinium ring in the crystals. The visible bands between 1330–1260 cm^{-1} correspond to the P–O(H) group, so it can be concluded that the hypodiphosphate anions are not completely deprotonated. In the frequency range 1120–910 cm^{-1} bands from the P–O functional group are visible, and in the range 700–430 cm^{-1} – O–P–O groups.

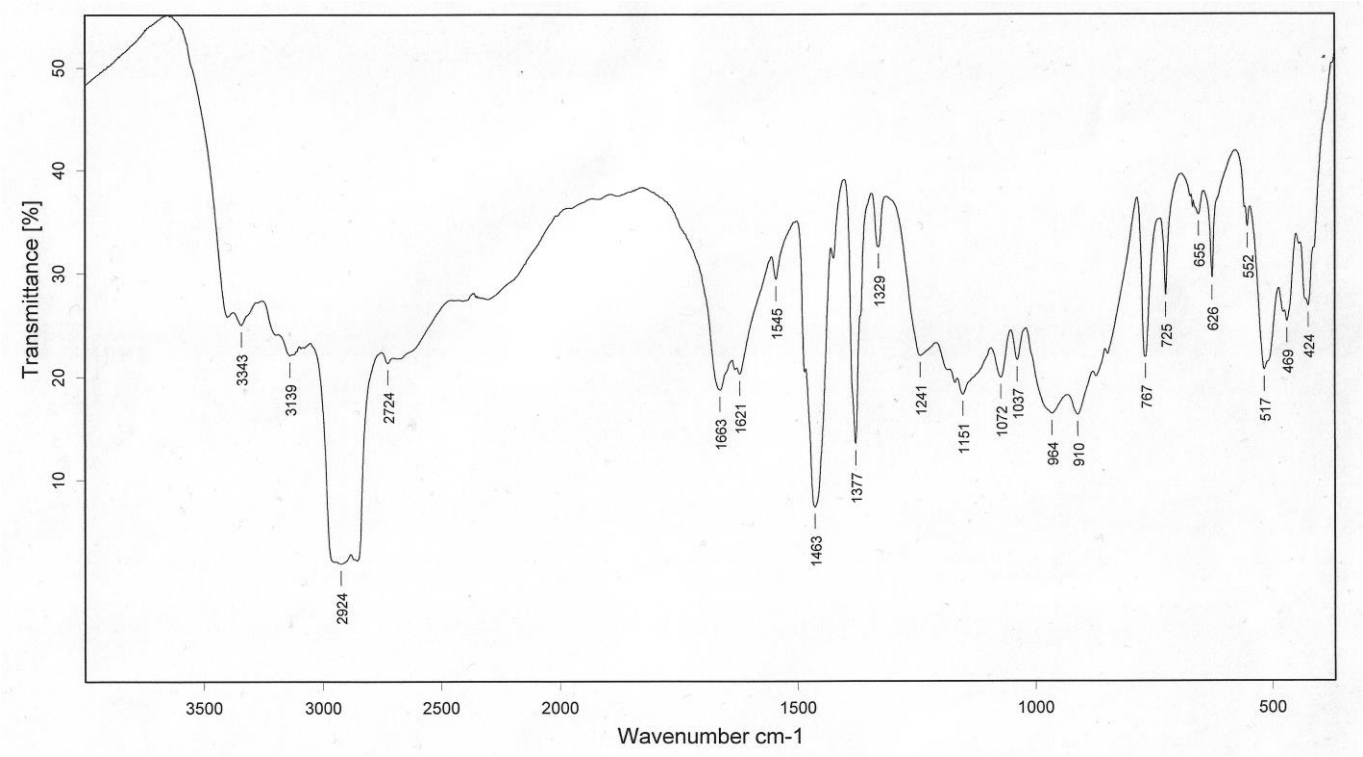


Figure S1. FT-IR spectrum of (**1**).

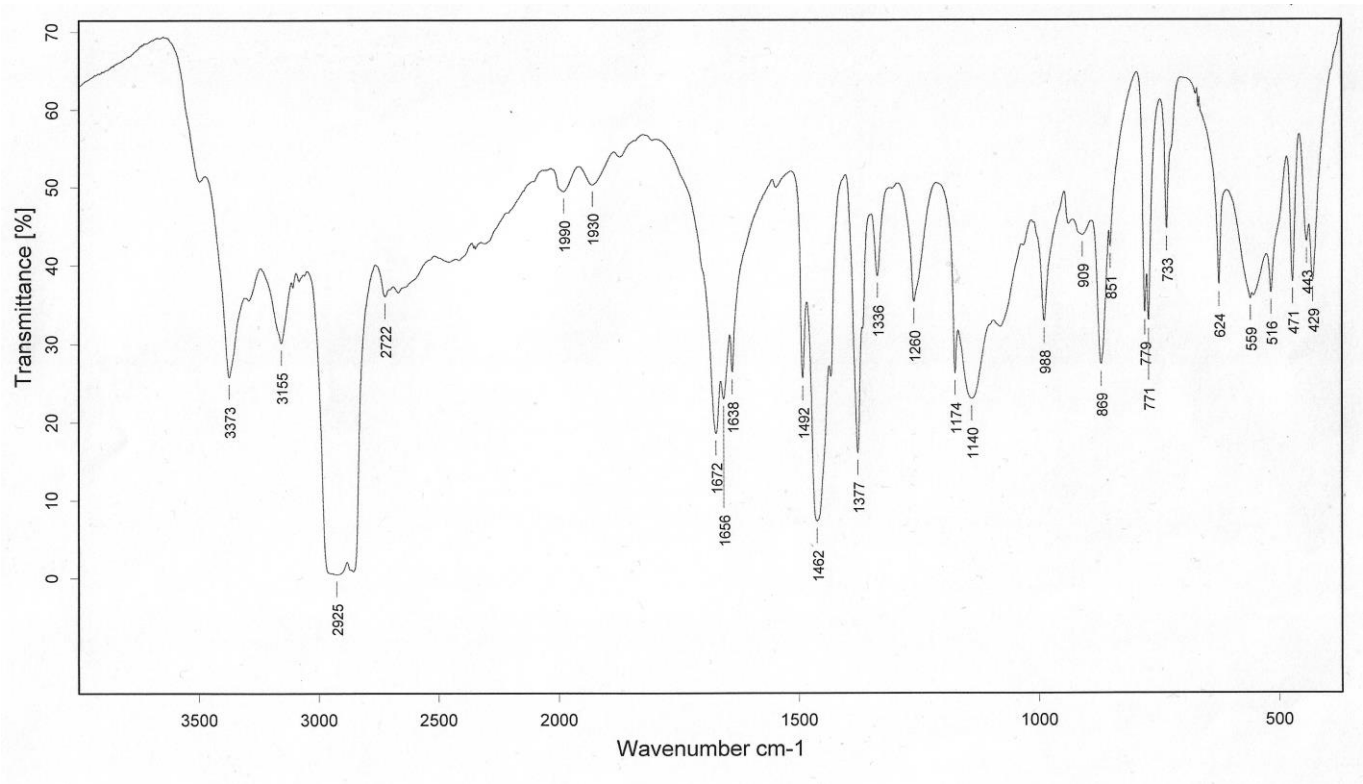


Figure S2. FT-IR spectrum of (**4**).

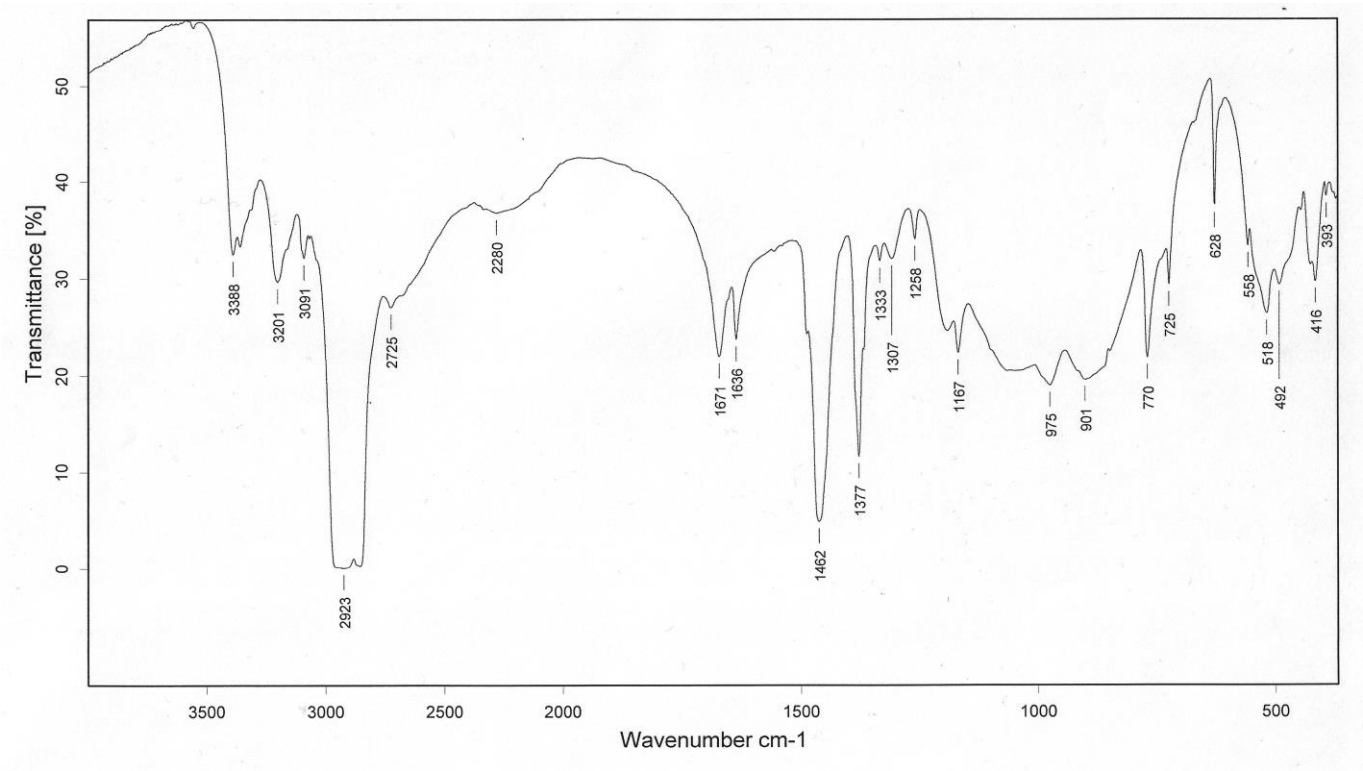


Figure S3. FT-IR spectrum of (**6**).

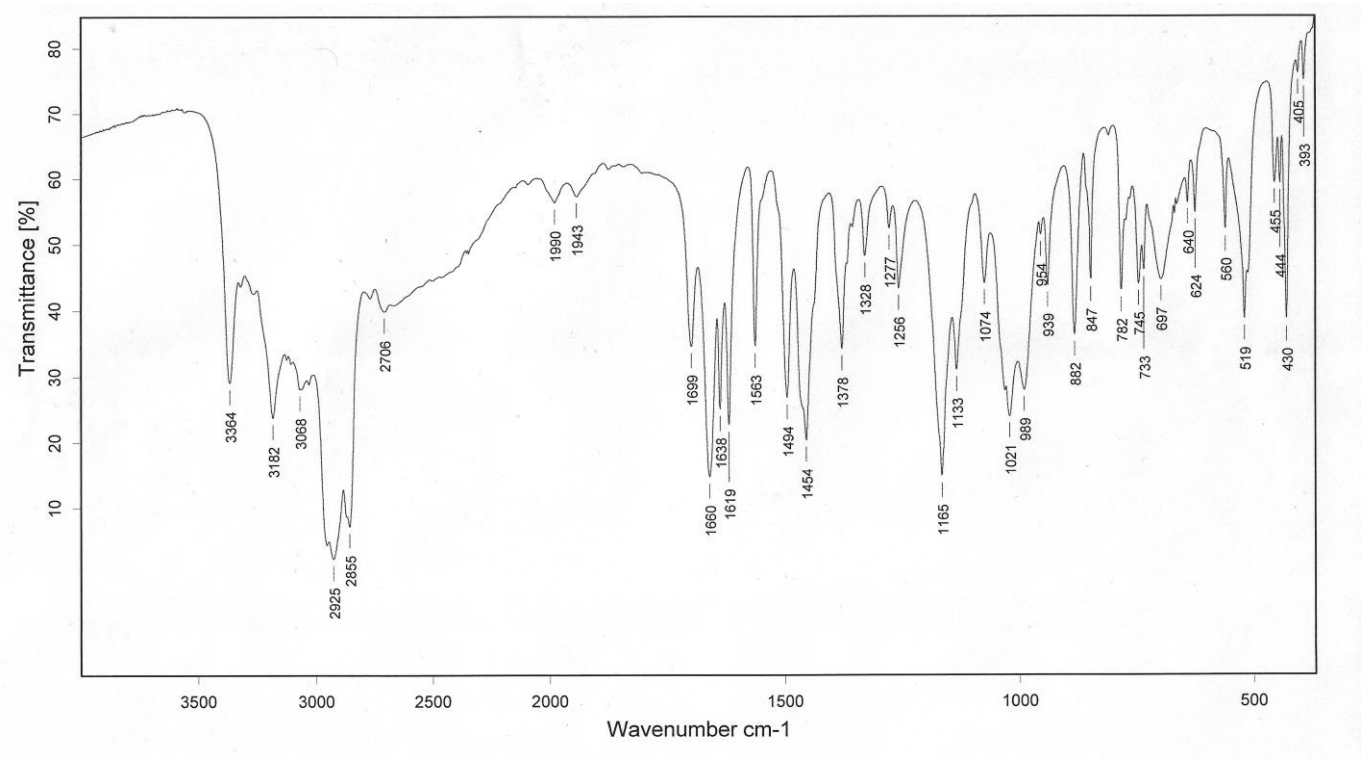
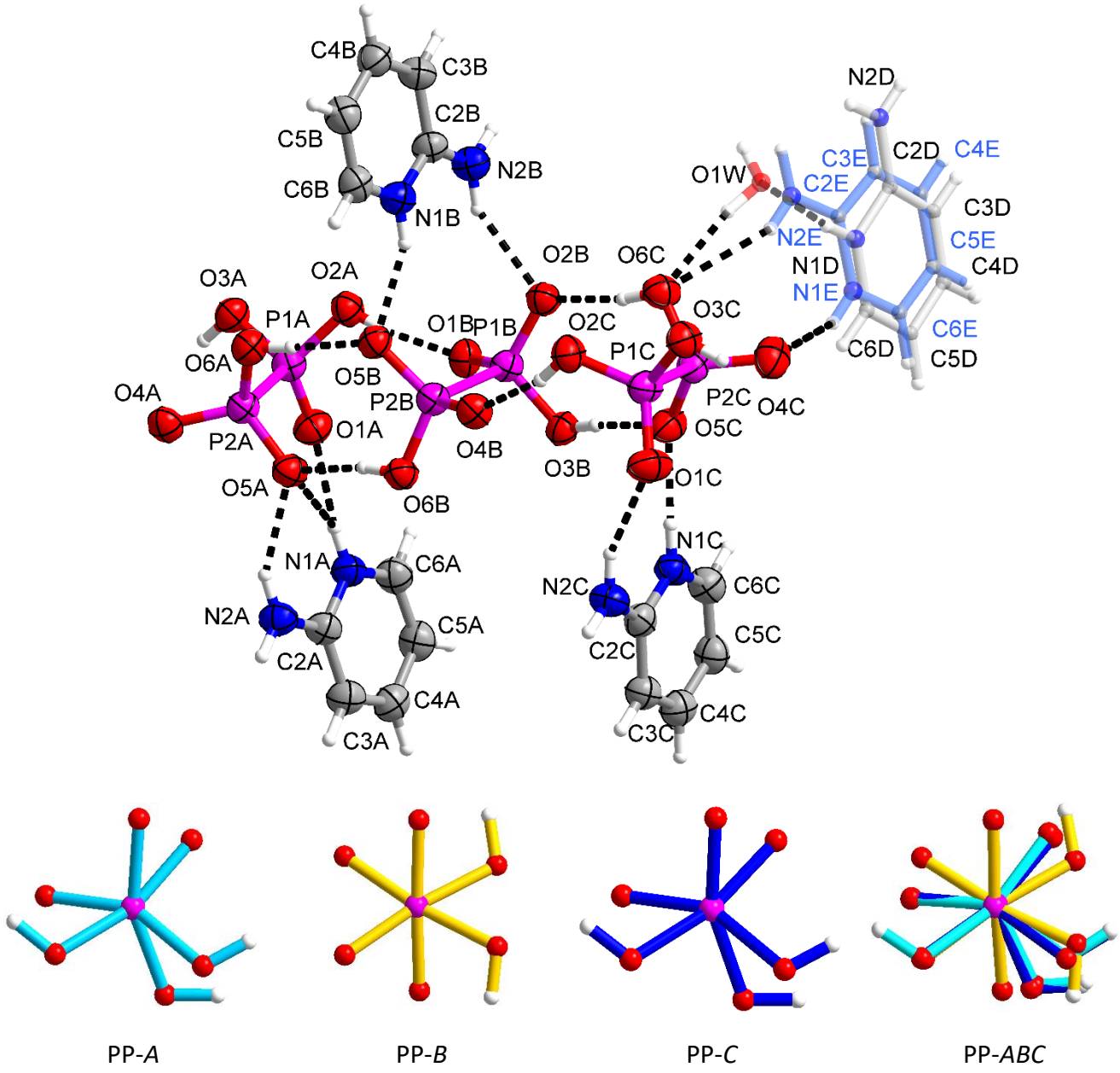
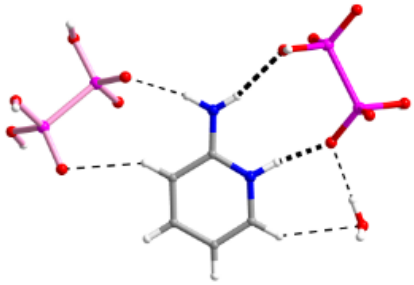


Figure S4. FT-IR spectrum of (**7**).

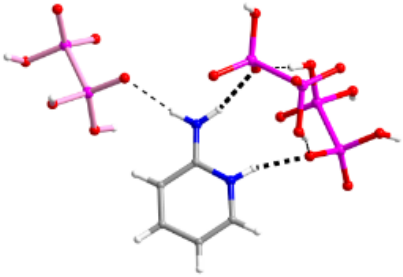


PP-*A* PP-*B* PP-*C* PP-*ABC*

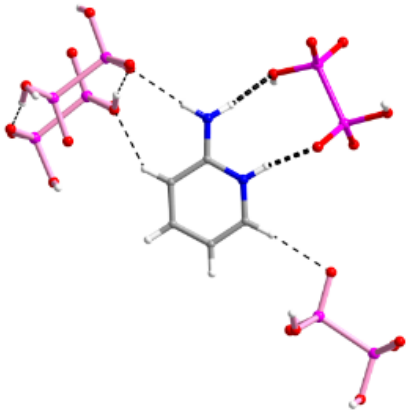
Figure S5. Asymmetric unit of (**2**) showing the atom-numbering scheme and symmetry-independent hydrogen bonds (dashed lines). Different positions of disordered 2-aminopyridiunium cation are shown with different colours (total SOF = 1). Displacement ellipsoids are shown at 50% probability level. The anions and a comparison of their conformation are shown at the bottom (the common reference points are the P1, P2 and O1 atoms). The yellow colour represents the dianions and the shades of blue – monoanions.



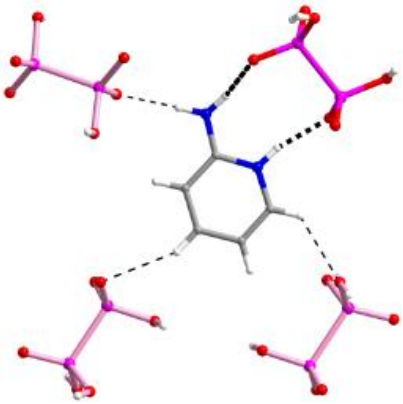
(**1**) 2-apH-*A*



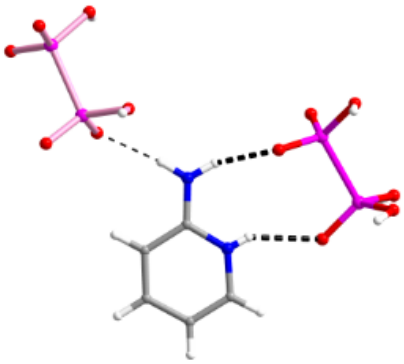
(**1**) 2-apH-*B*



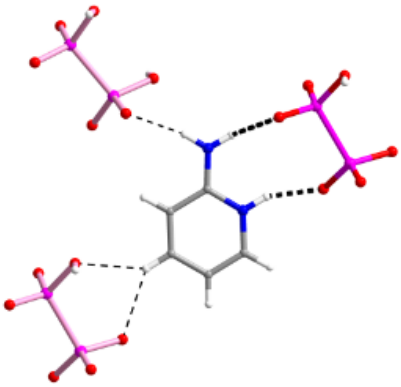
(**1**) 2-apH-*C*



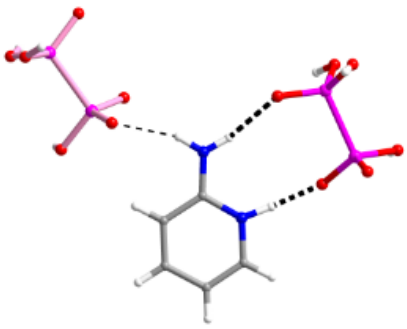
(**1**) 2-apH-*D*



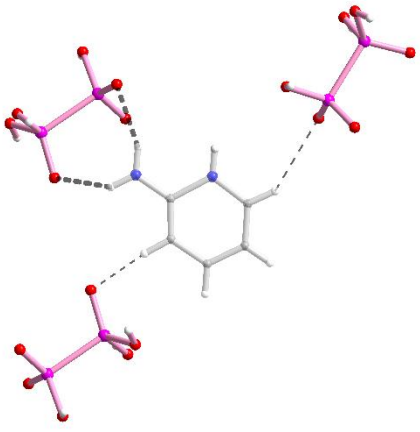
(**3**) 2-apH-*A*



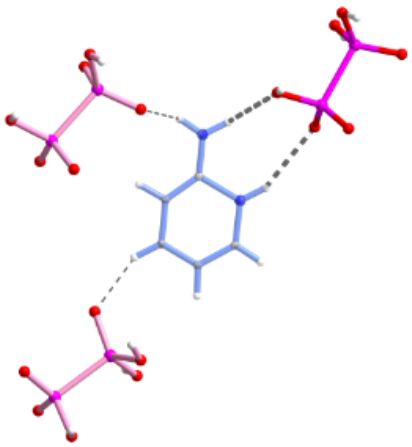
(**3**) 2-apH-*B*



(**3**) 2-apH-*C*

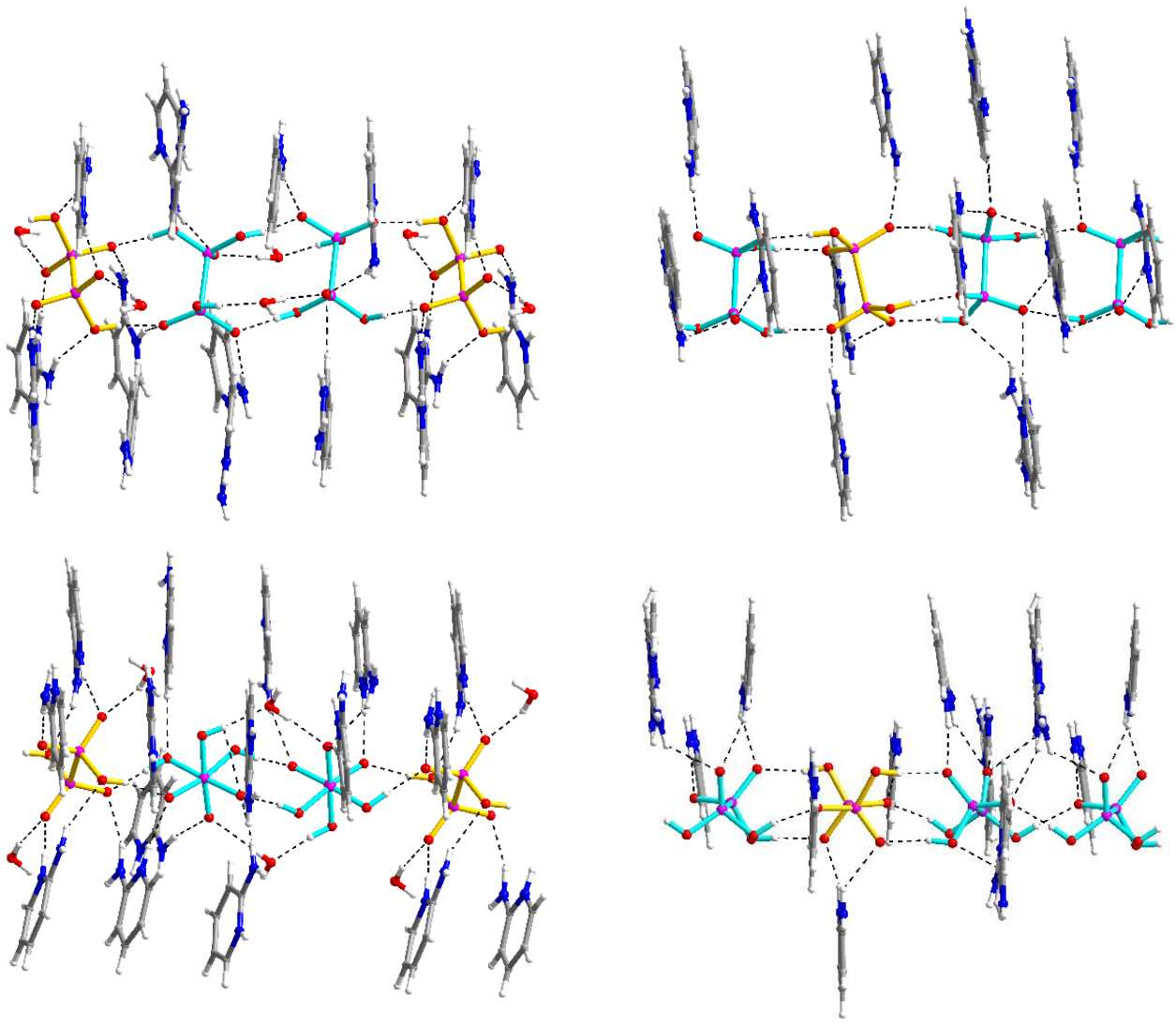


(**3**) 2-apH-*D* (75%)



(**3**) 2-apH-*D* (25%)

Figure S6. Hydrogen bond connections between the anions and the cations in the crystals of (**1**) and (**3**).



(**1**) (**3**)

Figure S7. The environment of the anions in crystals (**1**) and (**3**). Hydrogen bonds are shown with dashed lines. The turquoise colour represents monoanions and the yellow – dianions.

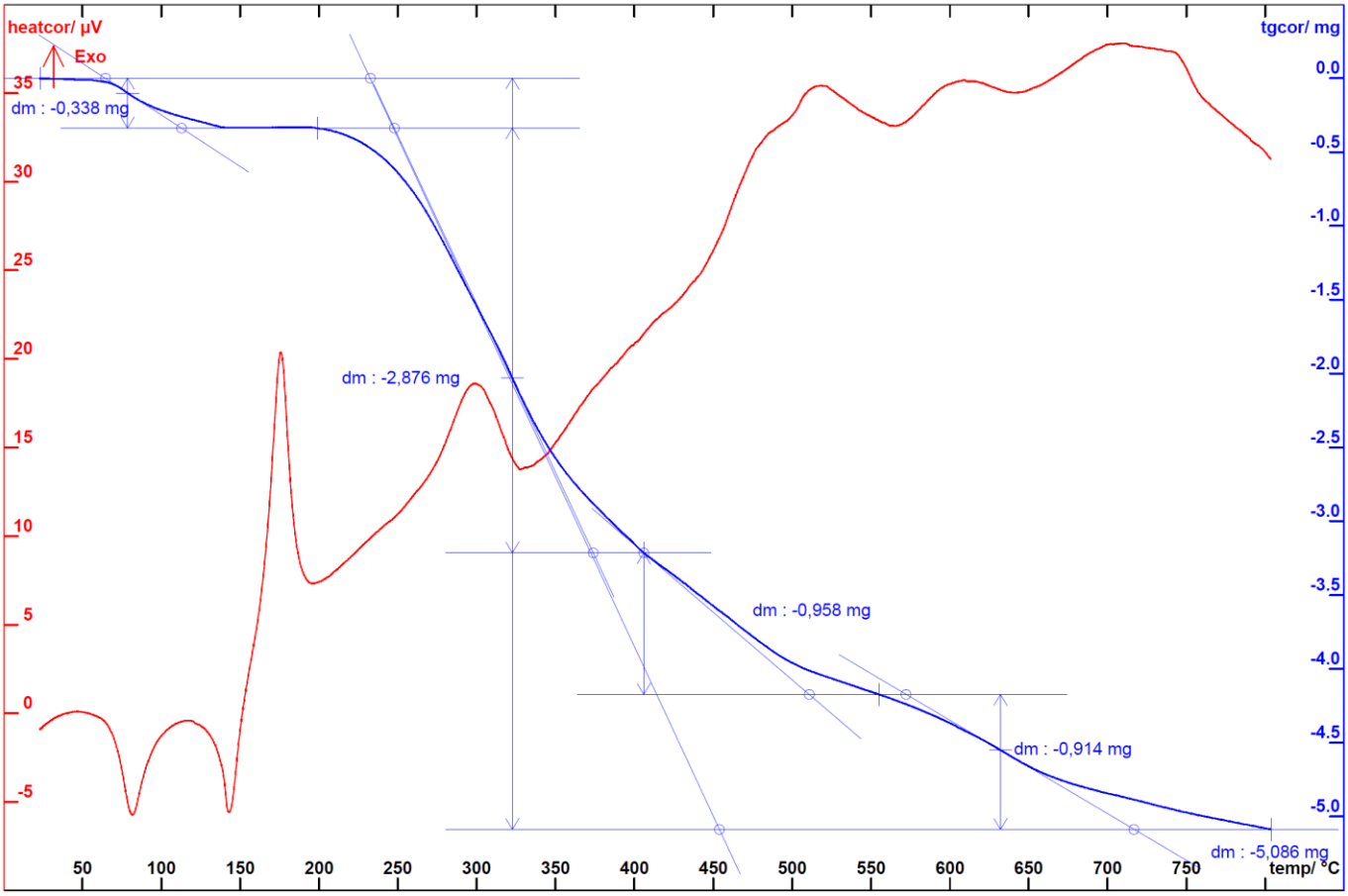


Figure S8. TGA/DTA curves for (**1**) (m = 9.606 mg).

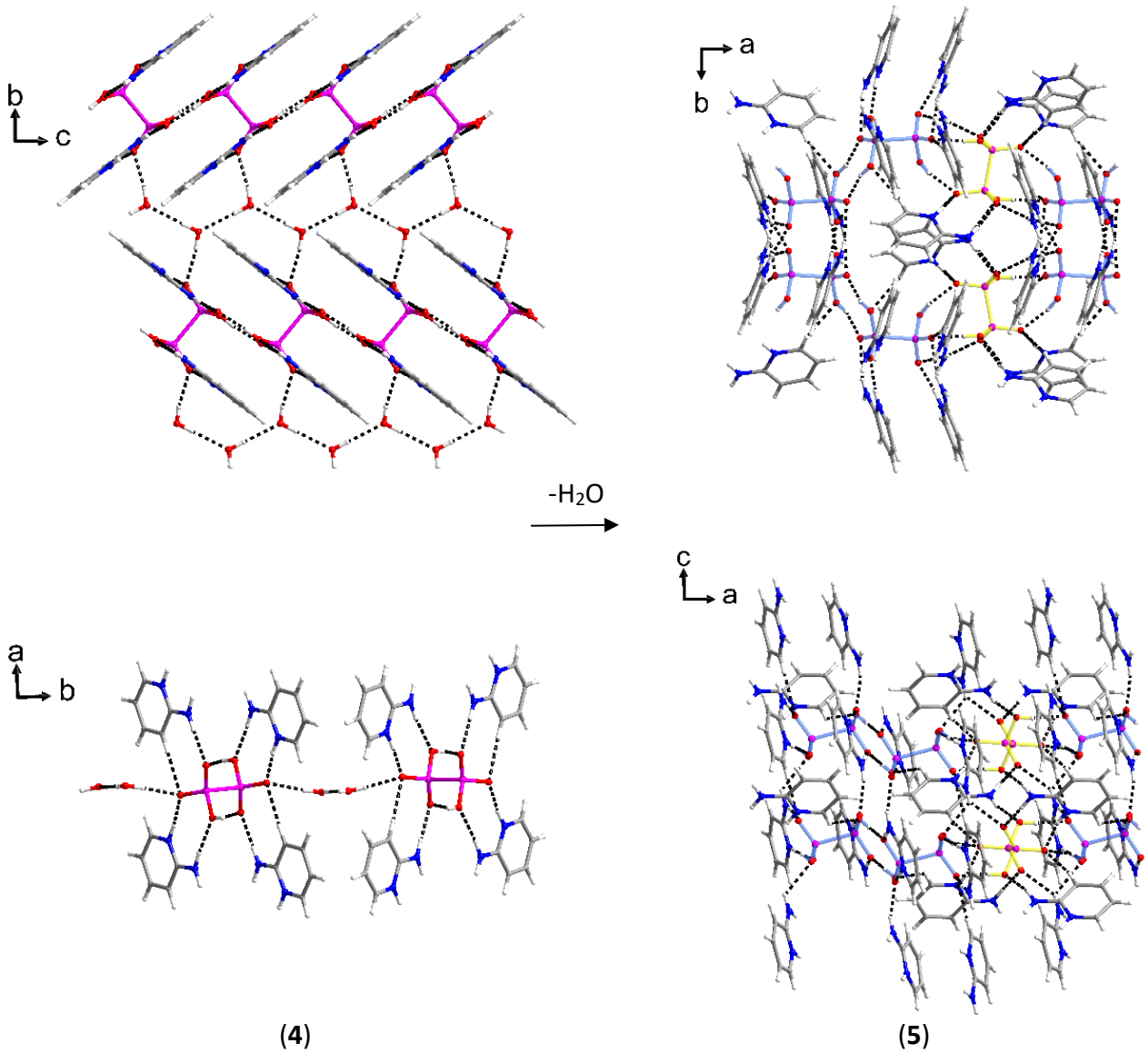
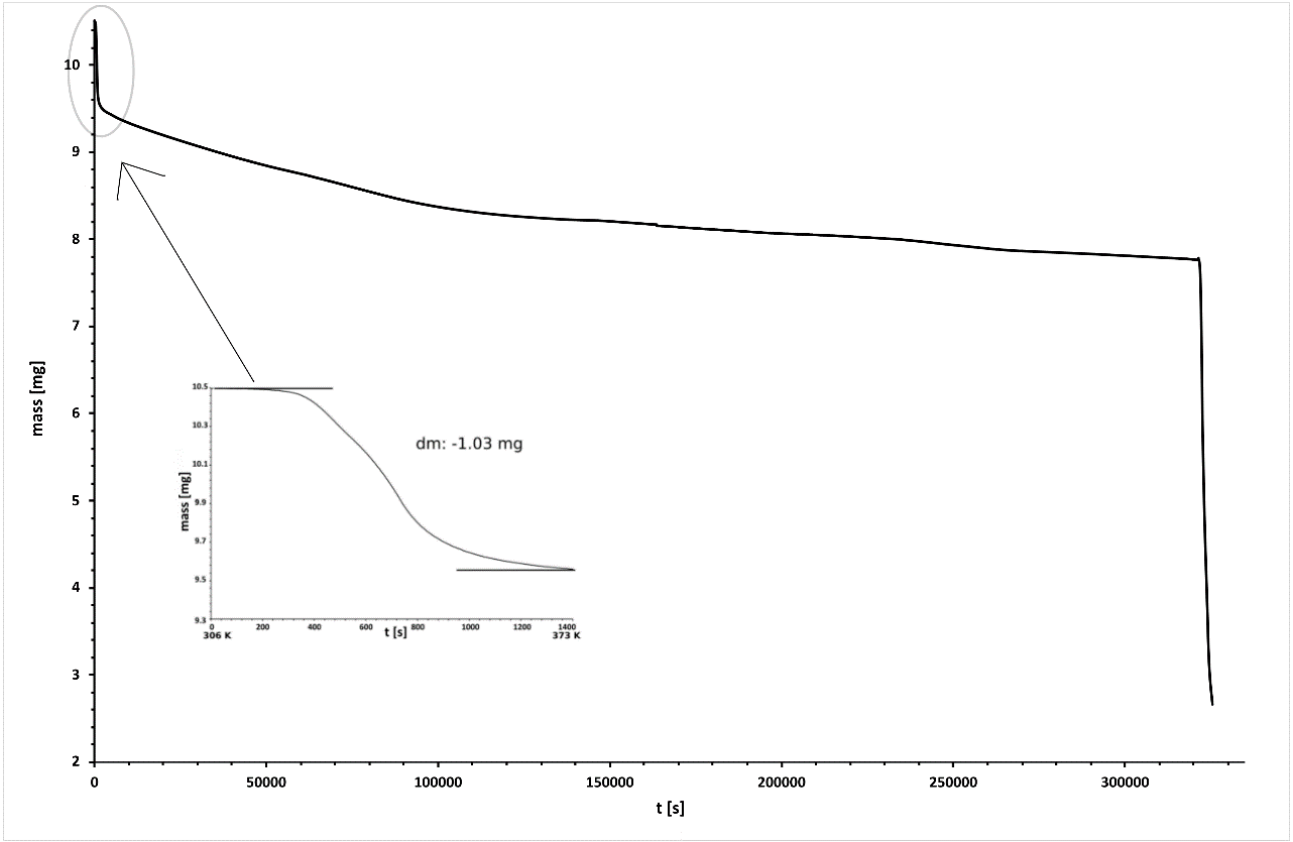
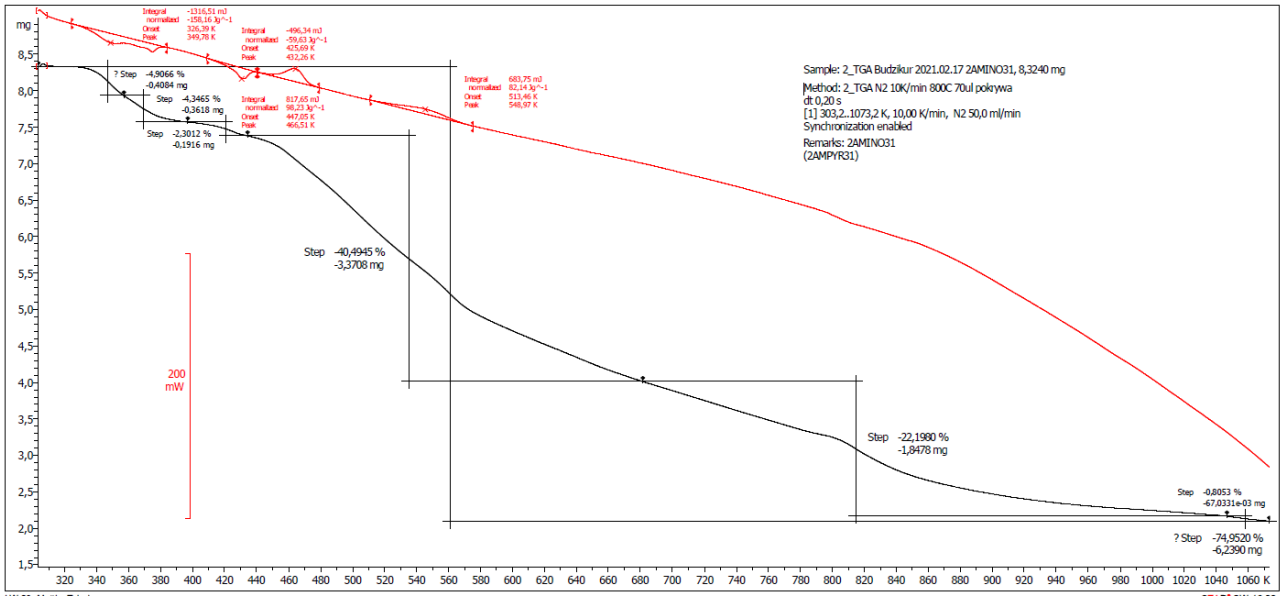


Figure S9. Crystal packing of (**4**) and (**5**). Hydrogen bonds are shown with dashed lines.



(a)



(b)

Figure S10. (a) TGA curve for (**4**) (m = 10.496 mg) shown as mass vs time. The measurement for 72 h was carried out in an isotherm at 378 K and then the sample was heated to 1073 K. The magnified area corresponds to the escape of water from the crystal. **(b)** TGA/DSC of (**4**) (m = 8.324 mg) shown as mass vs temperature.

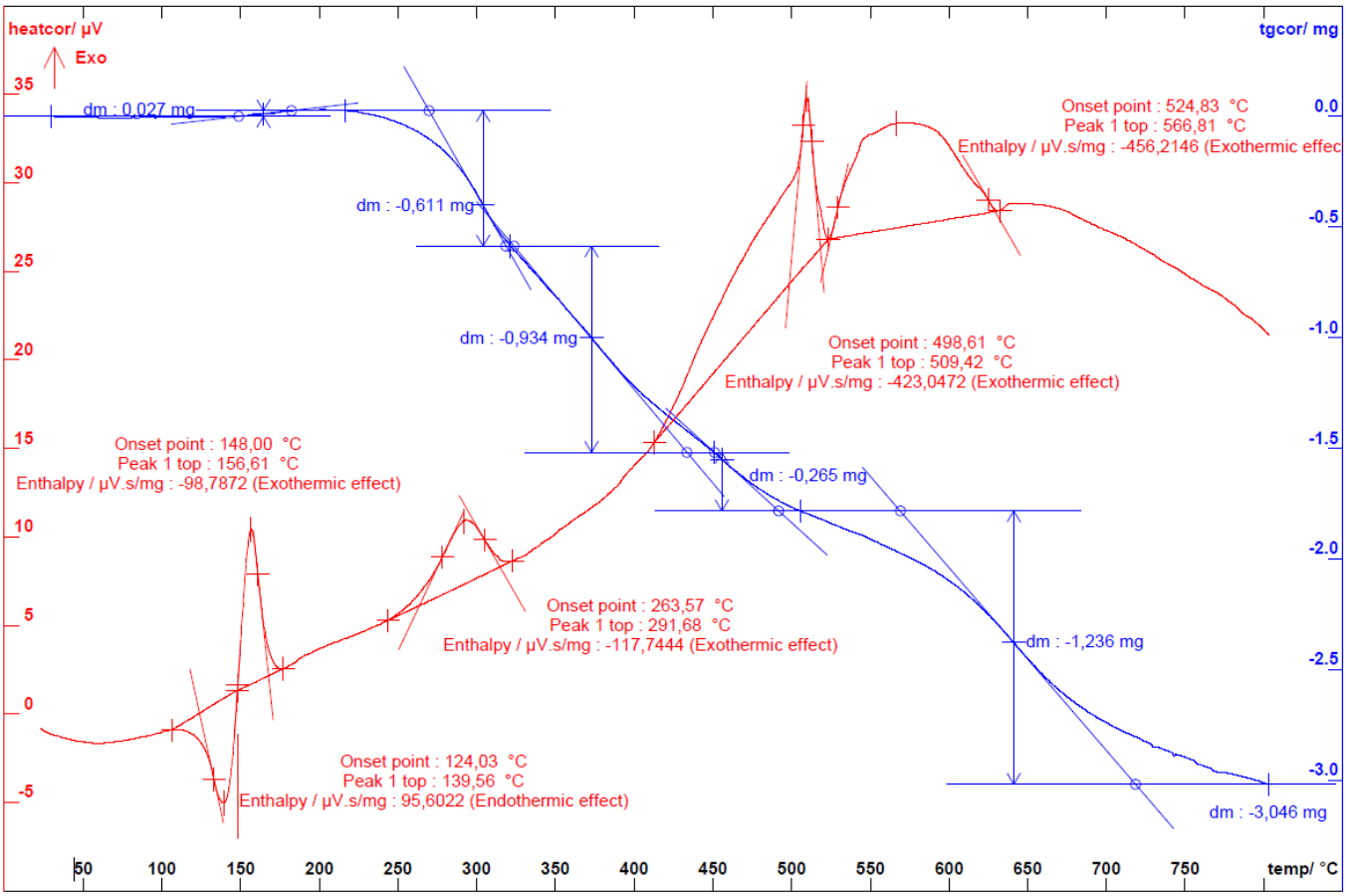


Figure S11. TGA/DTA curves for (**6**) (m = 5.538 mg).

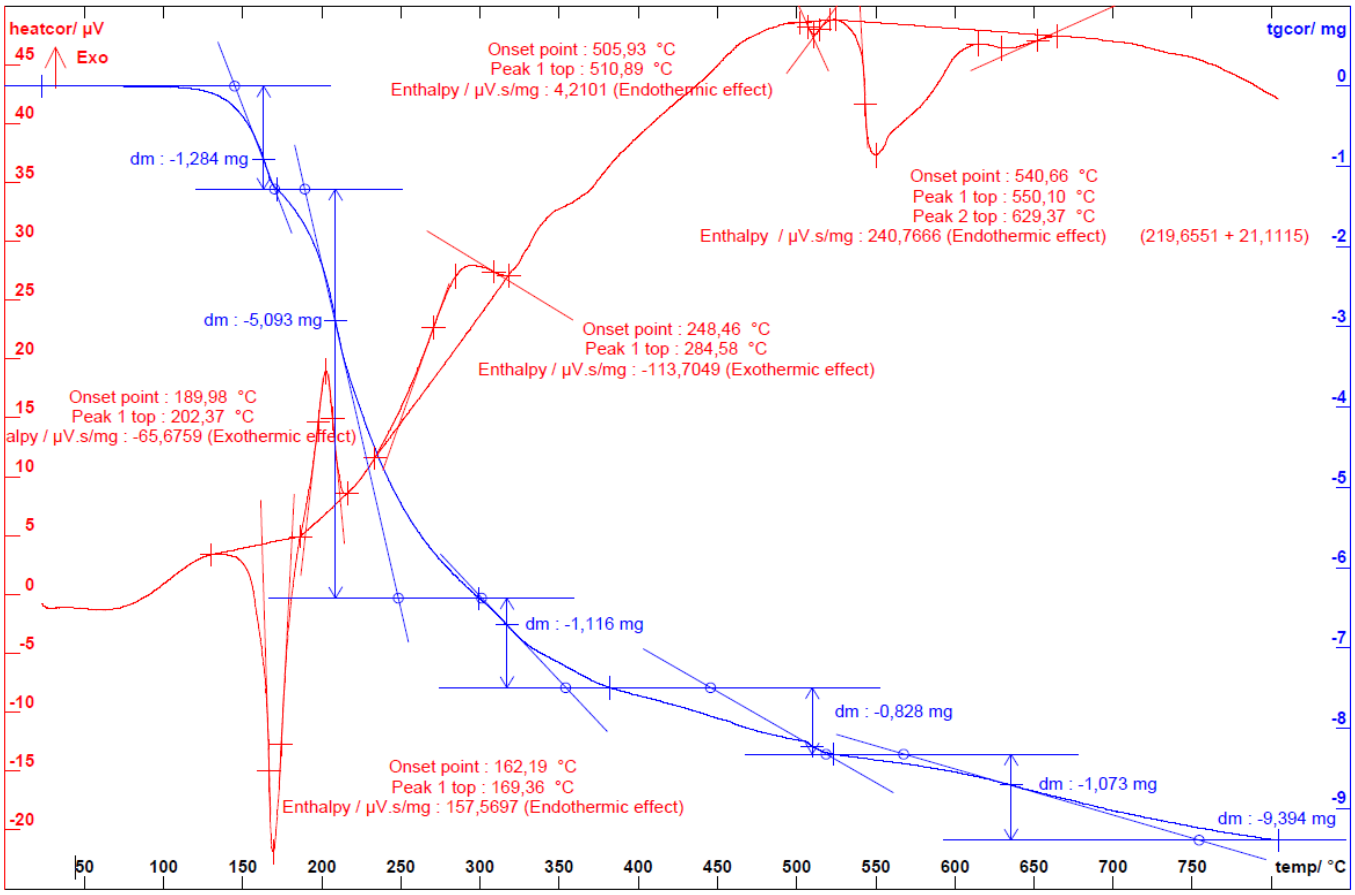


Figure S12. TGA/DTA curves for (**7**) (m = 12.6 mg).

Table S1. Selected geometric parameters (Å, °) for (**1**)

P1A—O1A	1.5030(11)	P2B—O4B	1.5062(12)
P1A—O2A	1.5096(12)	P2B—O5B	1.5093(12)
P1A—O3A	1.5807(12)	P2B—O6B	1.5700(12)
P1A—P2A	2.1790(6)	P1C—O1C	1.4936(12)
P2A—O4A	1.5019(12)	P1C—O2C	1.5484(12)
P2A—O5A	1.5088(12)	P1C—O3C	1.5544(12)
P2A—O6A	1.5844(12)	P1C—P2C	2.1810(6)
P1B—O1B	1.4968(12)	P2C—O4C	1.5091(12)
P1B—O2B	1.5468(12)	P2C—O5C	1.5117(12)
P1B—O3B	1.5555(12)	P2C—O6C	1.5618(12)
P1B—P2B	2.1815(6)		
O1A—P1A—O2A	115.77(7)	O4B—P2B—O5B	115.77(7)
O1A—P1A—O3A	110.91(6)	O4B—P2B—O6B	108.90(7)
O2A—P1A—O3A	107.42(7)	O5B—P2B—O6B	111.00(7)
O1A—P1A—P2A	108.55(5)	O4B—P2B—P1B	107.73(5)
O2A—P1A—P2A	108.78(5)	O5B—P2B—P1B	107.08(5)
O3A—P1A—P2A	104.84(5)	O6B—P2B—P1B	105.83(5)
O4A—P2A—O5A	116.69(7)	O1C—P1C—O2C	115.74(7)
O4A—P2A—O6A	111.75(7)	O1C—P1C—O3C	114.87(7)
O5A—P2A—O6A	106.44(7)	O2C—P1C—O3C	103.21(7)
O4A—P2A—P1A	108.78(5)	O1C—P1C—P2C	108.21(5)
O5A—P2A—P1A	109.27(5)	O2C—P1C—P2C	105.87(5)
O6A—P2A—P1A	103.02(5)	O3C—P1C—P2C	108.38(5)
O1B—P1B—O2B	115.19(7)	O4C—P2C—O5C	114.37(7)
O1B—P1B—O3B	114.65(7)	O4C—P2C—O6C	109.11(7)
O2B—P1B—O3B	103.58(7)	O5C—P2C—O6C	111.87(7)
O1B—P1B—P2B	109.82(5)	O4C—P2C—P1C	107.13(5)
O2B—P1B—P2B	105.28(5)	O5C—P2C—P1C	106.84(5)
O3B—P1B—P2B	107.62(5)	O6C—P2C—P1C	107.14(5)
O1A—P1A—P2A—O4A	−176.76(7)	O3B—P1B—P2B—O5B	−177.54(7)
O2A—P1A—P2A—O4A	56.48(7)	O1B—P1B—P2B—O6B	175.50(7)
O3A—P1A—P2A—O4A	−58.18(7)	O2B—P1B—P2B—O6B	50.93(7)
O1A—P1A—P2A—O5A	−48.33(7)	O3B—P1B—P2B—O6B	−59.07(7)
O2A—P1A—P2A—O5A	−175.09(7)	O1C—P1C—P2C—O4C	63.67(7)
O3A—P1A—P2A—O5A	70.24(7)	O2C—P1C—P2C—O4C	−171.66(7)
O1A—P1A—P2A—O6A	64.54(7)	O3C—P1C—P2C—O4C	−61.49(7)
O2A—P1A—P2A—O6A	−62.22(7)	O1C—P1C—P2C—O5C	−59.31(7)
O3A—P1A—P2A—O6A	−176.89(6)	O2C—P1C—P2C—O5C	65.36(7)
O1B—P1B—P2B—O4B	−68.12(7)	O3C—P1C—P2C—O5C	175.53(7)
O2B—P1B—P2B—O4B	167.30(7)	O1C—P1C—P2C—O6C	−179.35(7)
O3B—P1B—P2B—O4B	57.30(7)	O2C—P1C—P2C—O6C	−54.68(7)
O1B—P1B—P2B—O5B	57.03(7)	O3C—P1C—P2C—O6C	55.49(7)
O2B—P1B—P2B—O5B	−67.54(7)		

Table S2. Selected geometric parameters (Å, °) for (**3**)

P1A—O1A	1.483(5)	P2B—O4B	1.492(4)
P1A—O3A	1.549(5)	P2B—O5B	1.506(4)
P1A—O2A	1.551(5)	P2B—O6B	1.564(4)
P1A—P2A	2.192(2)	P1C—O1C	1.492(5)
P2A—O4A	1.491(5)	P1C—O2C	1.537(5)
P2A—O5A	1.504(4)	P1C—O3C	1.542(5)
P2A—O6A	1.571(5)	P1C—P2C	2.202(3)
P1B—O2B	1.502(5)	P2C—O4C	1.481(5)
P1B—O1B	1.509(4)	P2C—O5C	1.496(5)
P1B—O3B	1.553(4)	P2C—O6C	1.567(5)
P1B—P2B	2.196(2)		
O1A—P1A—O3A	115.6(3)	O4B—P2B—O5B	117.2(3)
O1A—P1A—O2A	116.4(3)	O4B—P2B—O6B	106.7(3)
O3A—P1A—O2A	101.7(3)	O5B—P2B—O6B	111.7(2)
O1A—P1A—P2A	106.8(2)	O4B—P2B—P1B	108.94(19)
O3A—P1A—P2A	108.3(2)	O5B—P2B—P1B	105.17(17)
O2A—P1A—P2A	107.6(2)	O6B—P2B—P1B	106.65(19)
O4A—P2A—O5A	115.1(3)	O1C—P1C—O2C	115.6(3)
O4A—P2A—O6A	109.7(3)	O1C—P1C—O3C	115.0(3)
O5A—P2A—O6A	110.6(3)	O2C—P1C—O3C	101.9(3)
O4A—P2A—P1A	109.0(2)	O1C—P1C—P2C	108.3(2)
O5A—P2A—P1A	104.5(2)	O2C—P1C—P2C	107.8(2)
O6A—P2A—P1A	107.46(19)	O3C—P1C—P2C	107.8(2)
O2B—P1B—O1B	116.8(3)	O4C—P2C—O5C	115.8(3)
O2B—P1B—O3B	110.9(3)	O4C—P2C—O6C	110.5(3)
O1B—P1B—O3B	106.2(3)	O5C—P2C—O6C	109.9(3)
O2B—P1B—P2B	105.47(19)	O4C—P2C—P1C	107.4(2)
O1B—P1B—P2B	109.3(2)	O5C—P2C—P1C	106.2(2)
O3B—P1B—P2B	107.89(19)	O6C—P2C—P1C	106.4(2)
O1A—P1A—P2A—O4A	−86.4(3)	O3B—P1B—P2B—O5B	−172.5(3)
O3A—P1A—P2A—O4A	38.7(3)	O2B—P1B—P2B—O6B	−172.3(3)
O2A—P1A—P2A—O4A	148.0(3)	O1B—P1B—P2B—O6B	61.4(3)
O1A—P1A—P2A—O5A	37.2(3)	O3B—P1B—P2B—O6B	−53.7(3)
O3A—P1A—P2A—O5A	162.3(3)	O1C—P1C—P2C—O4C	−83.4(3)
O2A—P1A—P2A—O5A	−88.5(3)	O2C—P1C—P2C—O4C	150.9(3)
O1A—P1A—P2A—O6A	154.7(3)	O3C—P1C—P2C—O4C	41.6(3)
O3A—P1A—P2A—O6A	−80.1(3)	O1C—P1C—P2C—O5C	41.1(3)
O2A—P1A—P2A—O6A	29.1(3)	O2C—P1C—P2C—O5C	−84.6(3)
O2B—P1B—P2B—O4B	−57.5(3)	O3C—P1C—P2C—O5C	166.1(3)
O1B—P1B—P2B—O4B	176.2(3)	O1C—P1C—P2C—O6C	158.2(3)
O3B—P1B—P2B—O4B	61.1(3)	O2C—P1C—P2C—O6C	32.5(3)
O2B—P1B—P2B—O5B	69.0(3)	O3C—P1C—P2C—O6C	−76.8(3)
O1B—P1B—P2B—O5B	−57.4(3)		

Table S3. Hydrogen-bond geometry (Å, °) for (**1**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*A*—H3*PA*···O4*C*^{i}	0.82(3)	1.74(3)	2.5547(16)	171(3)
O6*A*—H6*PA*···O4*B*	0.83(3)	1.74(3)	2.5620(17)	167(3)
O2*B*—H2*PB*···O5*C*	0.85(3)	1.62(3)	2.4616(17)	170(3)
O3*B*—H3*PB*···O2*A*	0.89(3)	1.61(3)	2.4988(16)	175(3)
O6*B*—H6*PB*···O1*W*	0.81(3)	1.80(3)	2.6115(17)	176(3)
O2*C*—H2*PC*···O5*B*	0.85(3)	1.65(3)	2.4978(17)	171(3)
O3*C*—H3*PC*···O5*A*^{ii}	0.86(3)	1.67(3)	2.5266(17)	176(3)
O6*C*—H6*PC*···O2*W*	0.86(3)	1.70(3)	2.5630(17)	174(3)
N1*A*—H1*NA*···O1*A*	0.91(2)	1.77(2)	2.6788(18)	171(2)
N2*A*—H2*A*1···O5*B*^{iii}	0.91(3)	2.01(3)	2.9013(19)	167(2)
N2*A*—H2*A*2···O6*A*	0.85(3)	2.23(3)	3.0385(19)	158(2)
C3*A*—H3*A*···O1*B*^{iii}	0.95	2.59	3.415(2)	145
N1*B*—H1*NB*···O4*B*	0.88(2)	1.93(2)	2.7846(18)	163(2)
N2*B*—H2*B*1···O2*A*	0.91(2)	1.99(2)	2.8669(19)	161(2)
N2*B*—H2*B*2···O1*B*^{iv}	0.89(3)	1.99(3)	2.8676(19)	169(2)
N1*C*—H1*NC*···O4*A*	0.87(2)	1.84(2)	2.7017(19)	166(2)
N2*C*—H2*C*1···O3*A*	0.91(3)	2.06(3)	2.934(2)	162(2)
N2*C*—H2*C*2···O5*C*^{v}	0.88(3)	2.23(3)	3.097(2)	168(2)
C3*C*—H3*C*···O2*B*^{v}	0.95	2.60	3.331(2)	134
C3*C*—H3*C*···O1*W*^{v}	0.95	2.64	3.320(2)	129
C6*C*—H6*C*···O1*C*^{vi}	0.95	2.33	3.272(2)	173
N1*D*—H1*ND*···O4*C*	0.87(3)	1.89(3)	2.7468(18)	166(2)
N2*D*—H2*D*1···O5*A*^{vi}	0.89(3)	1.99(3)	2.8811(19)	178(2)
N2*D*—H2*D*2···O1*C*	0.88(3)	2.10(3)	2.8878(19)	148(2)
C4*D*—H4*D*···O5*B*^{vii}	0.95	2.58	3.468(2)	155
C6*D*—H6*D*···O3*B*^{viii}	0.95	2.45	3.176(2)	134
O1*W*—H1*W*1···O4*A*^{vi}	0.84	2.03	2.8403(17)	161
O1*W*—H1*W*2···O1*C*	0.84	1.95	2.7861(17)	175
O2*W*—H2*W*1···O1*B*	0.84	1.99	2.8333(17)	178
O2*W*—H2*W*2···O1*A*^{iv}	0.84	1.93	2.7577(16)	169

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) *x*, *y*, *z*+1; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) −*x*+2, −*y*+1, −*z*+1; (v) *x*, −*y*+3/2, *z*−1/2; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) −*x*+1, *y*+1/2, −*z*+3/2; (viii) *x*, −*y*+3/2, *z*+1/2.

Table S4. Hydrogen-bond geometry (Å, °) for (**3**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*A*—H2*PA*···O1*B*	0.84	1.68	2.501(6)	166
O3*A*—H3*PA*···O4*C*^{i}	0.84	1.73	2.561(7)	172
O6*A*—H6*PA*···O5*B*	0.84	1.79	2.630(6)	174
O3*B*—H3*PB*···O5*C*	0.84	1.73	2.559(6)	170
O6*B*—H6*PB*···O5*A*	0.84	1.70	2.528(6)	169
O2*C*—H2*PC*···O4*B*	0.84	1.68	2.496(6)	162
O3*C*—H3*PC*···O4*A*^{ii}	0.84	1.71	2.547(7)	174
O6*C*—H6*PC*···O2*B*	0.84	1.75	2.586(7)	171
N1*A*—H1*NA*···O1*A*	0.88	2.08	2.792(7)	138
N1*A*—H1*NA*···O5*A*	0.88	2.53	3.222(7)	136
N2*A*—H2*A*1···O5*A*	0.88	1.98	2.797(7)	153
N2*A*—H2*A*2···O4*B*^{iii}	0.88	2.02	2.884(7)	169
N1*B*—H1*NB*···O5*B*	0.88	1.93	2.741(7)	153
N2*B*—H2*B*1···O2*B*	0.88	2.14	2.886(7)	142
N2*B*—H2*B*2···O1*B*^{iv}	0.88	2.04	2.899(7)	165
N1*C*—H1*NC*···O5*C*	0.88	1.81	2.669(7)	164
N2*C*—H2*C*1···O1*C*	0.88	2.13	2.950(7)	155
N2*C*—H2*C*2···O4*A*^{iii}	0.88	2.06	2.903(7)	160
C3*C*—H3*C*···O4*A*^{iii}	0.95	2.62	3.350(8)	134
N1*D*—H1*ND*···O1*W*	0.88	1.79	2.67(5)	171
N2*D*—H2*D*1···O1*C*^{v}	0.88	2.49	3.111(11)	128
N2*D*—H2*D*2···O4*C*^{v}	0.88	2.30	3.058(11)	145
C3*D*—H3*D*···O1*C*^{vi}	0.95	2.05	2.999(11)	174
C5*D*—H5*D*···O3*A*^{vii}	0.95	2.58	3.418(13)	147
C6*D*—H6*D*···O1*W*^{viii}	0.95	2.50	3.11(4)	121
N1*E*—H1*NE*···O4*C*	0.88	2.49	3.30(3)	153
N2*E*—H2*E*1···O1*A*^{iv}	0.88	2.24	2.93(3)	135
N2*E*—H2*E*2···O6*C*	0.88	2.46	3.11(3)	132
O1*W*—H1*W*1···O6*C*	0.84	1.98	2.71(4)	146
O1*W*—H1*W*2···O1*A*^{iv}	0.84	1.96	2.76(4)	159

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, *y*+1/2, −*z*+1/2; (v) −*x*+2, *y*+1/2, −*z*+1/2; (vi) *x*, −*y*+3/2, *z*−1/2; (vii) −*x*+1, *y*−1/2, −*z*+1/2; (viii) −*x*+2, *y*−1/2, −*z*+1/2.

Table S5. Selected geometric parameters (Å, °) for (**4**)

P1—O1	1.5096(19)	P1—O3	1.577(2)
P1—O2	1.513(2)	P1—P1^{i}	2.1754(14)
O1—P1—O2	115.27(11)	O1—P1—P1^{i}	108.21(9)
O1—P1—O3	107.96(11)	O2—P1—P1^{i}	108.02(9)
O2—P1—O3	112.47(11)	O3—P1—P1^{i}	104.26(9)
O1—P1—P1^{i}—O1^{i}	180	O3—P1—P1^{i}—O2^{i}	60.17(13)
O2—P1—P1^{i}—O1^{i}	54.58(13)	O1—P1—P1^{i}—O3^{i}	65.25(13)
O3—P1—P1^{i}—O1^{i}	−65.25(13)	O2—P1—P1^{i}—O3^{i}	−60.17(13)
O1—P1—P1^{i}—O2^{i}	−54.58(13)	O3—P1—P1^{i}—O3^{i}	180
O2—P1—P1^{i}—O2^{i}	180		

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

Table S6. Selected geometric parameters (Å, °) for (**5**)

P1A—O3A	1.512(5)	P2A—O4A	1.573(5)
P1A—O2A	1.525(5)	P1B—O3B	1.499(5)
P1A—O1A	1.549(5)	P1B—O2B	1.514(5)
P1A—P2A	2.185(3)	P1B—O1B	1.566(5)
P2A—O6A	1.503(5)	P1B—P1B^{i}	2.177(4)
P2A—O5A	1.516(5)		
O3A—P1A—O2A	113.2(3)	O6A—P2A—P1A	105.6(2)
O3A—P1A—O1A	109.8(3)	O5A—P2A—P1A	110.5(2)
O2A—P1A—O1A	112.2(3)	O4A—P2A—P1A	102.9(2)
O3A—P1A—P2A	105.5(2)	O3B—P1B—O2B	115.5(3)
O2A—P1A—P2A	107.4(2)	O3B—P1B—O1B	112.0(3)
O1A—P1A—P2A	108.5(2)	O2B—P1B—O1B	107.0(3)
O6A—P2A—O5A	115.8(3)	O3B—P1B—P1B^{i}	110.5(2)
O6A—P2A—O4A	110.0(3)	O2B—P1B—P1B^{i}	106.7(2)
O5A—P2A—O4A	111.2(3)	O1B—P1B—P1B^{i}	104.5(2)
O3A—P1A—P2A—O6A	−67.7(3)	O1B—P1B—P1B^{i}—O1B^{i}	180
O2A—P1A—P2A—O6A	53.3(3)	O2B—P1B—P1B^{i}—O1B^{i}	−66.9(3)
O1A—P1A—P2A—O6A	174.7(3)	O3B—P1B—P1B^{i}—O1B^{i}	59.3(3)
O3A—P1A—P2A—O5A	58.2(3)	O1B—P1B—P1B^{i}—O2B^{i}	66.9(3)
O2A—P1A—P2A—O5A	179.2(3)	O2B—P1B—P1B^{i}—O2B^{i}	180
O1A—P1A—P2A—O5A	−59.4(3)	O3B—P1B—P1B^{i}—O2B^{i}	−53.8(4)
O3A—P1A—P2A—O4A	177.0(3)	O1B—P1B—P1B^{i}—O3B^{i}	−59.3(3)
O2A—P1A—P2A—O4A	−62.1(3)	O2B—P1B—P1B^{i}—O3B^{i}	53.8(4)
O1A—P1A—P2A—O4A	59.3(3)	O3B—P1B—P1B^{i}—O3B^{i}	180

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.

Table S7. Hydrogen-bond geometry (Å, °) for (**4**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*P*···O2^{ii}	0.81(5)	1.72(5)	2.522(3)	169(5)
N1—H1*N*···O1	0.93(4)	1.73(4)	2.658(3)	173(3)
N2—H2*N*1···O3	0.90(4)	2.18(4)	3.074(4)	173(3)
N2—H2*N*2···O2^{iii}	0.87(4)	2.04(4)	2.900(3)	171(3)
C3—H3···O1^{iii}	0.95	2.44	3.377(4)	168
O1*W*—H1*W*1···O1	0.84	1.98	2.811(3)	170
O1*W*—H1*W*2···O1*W*^{iv}	0.84	2.05	2.8922(19)	178

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

Table S8. Hydrogen-bond geometry (Å, °) for (**5**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*PA*···O2*A*^{ii}	0.84	1.71	2.517(6)	160
O4*A*—H4*PA*···O2*B*^{i}	0.84	1.84	2.627(6)	155
O1*B*—H1*PB*···O5*A*	0.84	1.73	2.567(6)	173
N1*A*—H1*NA*···O3*A*	0.88	1.80	2.672(7)	174
N2*A*—H2*A*2···O3*A*^{iii}	0.88	1.95	2.763(8)	153
N2*A*—H2*A*1···O2*A*	0.88	2.20	3.052(7)	162
C3*A*—H3*A*···O1*A*^{iii}	0.95	2.52	3.436(9)	161
N1*B*—H1*NB*···O6*A*	0.88	1.83	2.702(9)	174
N2*B*—H2*B*2···O6*A*^{iv}	0.88	2.42	3.000(9)	124
N2*B*—H2*B*1···O5*A*	0.88	2.18	3.038(9)	166
C6*B*—H6*B*···O5*A*^{iii}	0.95	2.41	3.350(10)	173
N1*C*—H1*NC*···O2*B*	0.88	1.83	2.688(8)	163
N2*C*—H2*C*2···O1*B*^{iii}	0.88	2.14	3.004(8)	166
N2*C*—H2*C*1···O3*B*	0.88	1.95	2.820(9)	170
C3*C*—H3*C*···O2*B*^{iii}	0.95	2.20	3.119(9)	164
C6*C*—H6*C*···O1*A*^{i}	0.95	2.41	3.137(9)	133

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

Table S9. Selected geometric parameters (Å, °) for (**6**)

P1A—O1A	1.5167(15)	P1B—O1B	1.4894(15)
P1A—O2A	1.5192(14)	P1B—O2B	1.5425(15)
P1A—O3A	1.5579(16)	P1B—O3B	1.5515(16)
P1A—P1A^{i}	2.1750(11)	P1B—P1B^{ii}	2.1748(12)
O1A—P1A—O2A	114.30(8)	O1B—P1B—O2B	116.13(9)
O1A—P1A—O3A	113.99(8)	O1B—P1B—O3B	112.85(8)
O2A—P1A—O3A	108.45(8)	O2B—P1B—O3B	105.95(8)
O1A—P1A—P1A^{i}	106.62(7)	O1B—P1B—P1B^{ii}	110.06(7)
O2A—P1A—P1A^{i}	107.04(7)	O2B—P1B—P1B^{ii}	105.73(7)
O3A—P1A—P1A^{i}	105.86(7)	O3B—P1B—P1B^{ii}	105.33(7)
O1A—P1A—P1A^{i}—O1A^{i}	180	O1B—P1B—P1B^{ii}—O1B^{ii}	180
O2A—P1A—P1A^{i}—O1A^{i}	57.27(9)	O2B—P1B—P1B^{ii}—O1B^{ii}	−53.84(10)
O3A—P1A—P1A^{i}—O1A^{i}	−58.27(9)	O3B—P1B—P1B^{ii}—O1B^{ii}	58.08(10)
O1A—P1A—P1A^{i}—O2A^{i}	−57.27(9)	O1B—P1B—P1B^{ii}—O2B^{ii}	53.84(10)
O2A—P1A—P1A^{i}—O2A^{i}	180	O2B—P1B—P1B^{ii}—O2B^{ii}	180
O3A—P1A—P1A^{i}—O2A^{i}	64.45(9)	O3B—P1B—P1B^{ii}—O2B^{ii}	−68.08(9)
O1A—P1A—P1A^{i}—O3A^{i}	58.27(9)	O1B—P1B—P1B^{ii}—O3B^{ii}	−58.08(10)
O2A—P1A—P1A^{i}—O3A^{i}	−64.45(9)	O2B—P1B—P1B^{ii}—O3B^{ii}	68.08(9)
O3A—P1A—P1A^{i}—O3A^{i}	180	O3B—P1B—P1B^{ii}—O3B^{ii}	180

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

Table S10. Selected geometric parameters (Å, °) for (**7**)

P1—O1	1.5018(14)	P1—O3	1.5788(14)
P1—O2	1.5195(13)	P1—P1^{i}	2.1824(9)
O1—P1—O2	117.21(8)	O1—P1—P1^{i}	108.98(6)
O1—P1—O3	111.76(8)	O2—P1—P1^{i}	106.56(6)
O2—P1—O3	106.64(7)	O3—P1—P1^{i}	104.89(6)
O1—P1—P1^{i}—O1^{i}	180	O3—P1—P1^{i}—O2^{i}	−67.16(8)
O2—P1—P1^{i}—O1^{i}	−52.65(9)	O1—P1—P1^{i}—O3^{i}	−60.19(8)
O3—P1—P1^{i}—O1^{i}	60.19(8)	O2—P1—P1^{i}—O3^{i}	67.16(8)
O1—P1—P1^{i}—O2^{i}	52.65(9)	O3—P1—P1^{i}—O3^{i}	180
O2—P1—P1^{i}—O2^{i}	180		

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.

Table S11. Hydrogen-bond geometry (Å, °) for (**6**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*A*—H3*PA*···O1*B*^{ii}	0.84	1.70	2.536(2)	174
O2*B*—H2*PB*···O2*A*^{iii}	0.84	1.69	2.528(2)	175
O3*B*—H3*PB*···O1*A*	0.84	1.62	2.459(2)	172
N1—H1*N*···O2*A*	0.78(3)	1.99(3)	2.769(3)	179(3)
N2—H2*N*1···O1*A*	0.83(3)	2.17(3)	2.993(3)	173(3)
N2—H2*N*2···O3*B*^{iv}	0.91(3)	2.04(3)	2.941(3)	180(3)
C6—H6···O2*A*^{v}	0.95	2.56	3.372(3)	144

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

Table S12. Hydrogen-bond geometry (Å, °) for (**7**)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*P*···N1*B*	0.83(3)	1.83(3)	2.640(2)	168(3)
N1*A*—H1*NA*···O2	0.86(4)	1.83(4)	2.682(2)	174(3)
N2*A*—H2*A*1···O2^{ii}	0.94(3)	1.91(3)	2.833(2)	167(3)
N2*A*—H2*A*2···O1^{i}	0.88(3)	1.98(4)	2.833(2)	163(3)
N2*B*—H2*B*1···O1^{iii}	0.93(3)	1.95(3)	2.864(2)	170(2)
N2*B*—H2*B*2···O2^{i}	0.89(3)	2.13(3)	2.962(2)	157(2)

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