Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis, structural characterization and computational studies of layered metal phosphonates: $[M(HO_3P–C_5H_4N–PO_3H)_2(H_2O)_2]_n$ [M^{II} = Co, Zn, Cd]

Magdalena Wilk,*[a] Katarzyna N. Jarzembska,[b] Jan Janczak,[c] Marek Duczmal,[a] Józef Hoffmann[a] and Veneta Videnova-Adrabinska*[a]

[a] *Department of Chemistry, Wrocław University of Technology, 27 Wybrzeże Wyspiańskiego St., 50-370 Wrocław, Poland. E-mail: magdalena.wilk@pwr.edu.pl, Veneta.Videnova-Adrabinska@pwr.edu.pl*

[b] *Department of Chemistry, University of Warsaw, 1 Pasteura St., 02-093 Warsaw, Poland.*

[c] *Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 2 Okólna St., 50-950 Wrocław, Poland.*

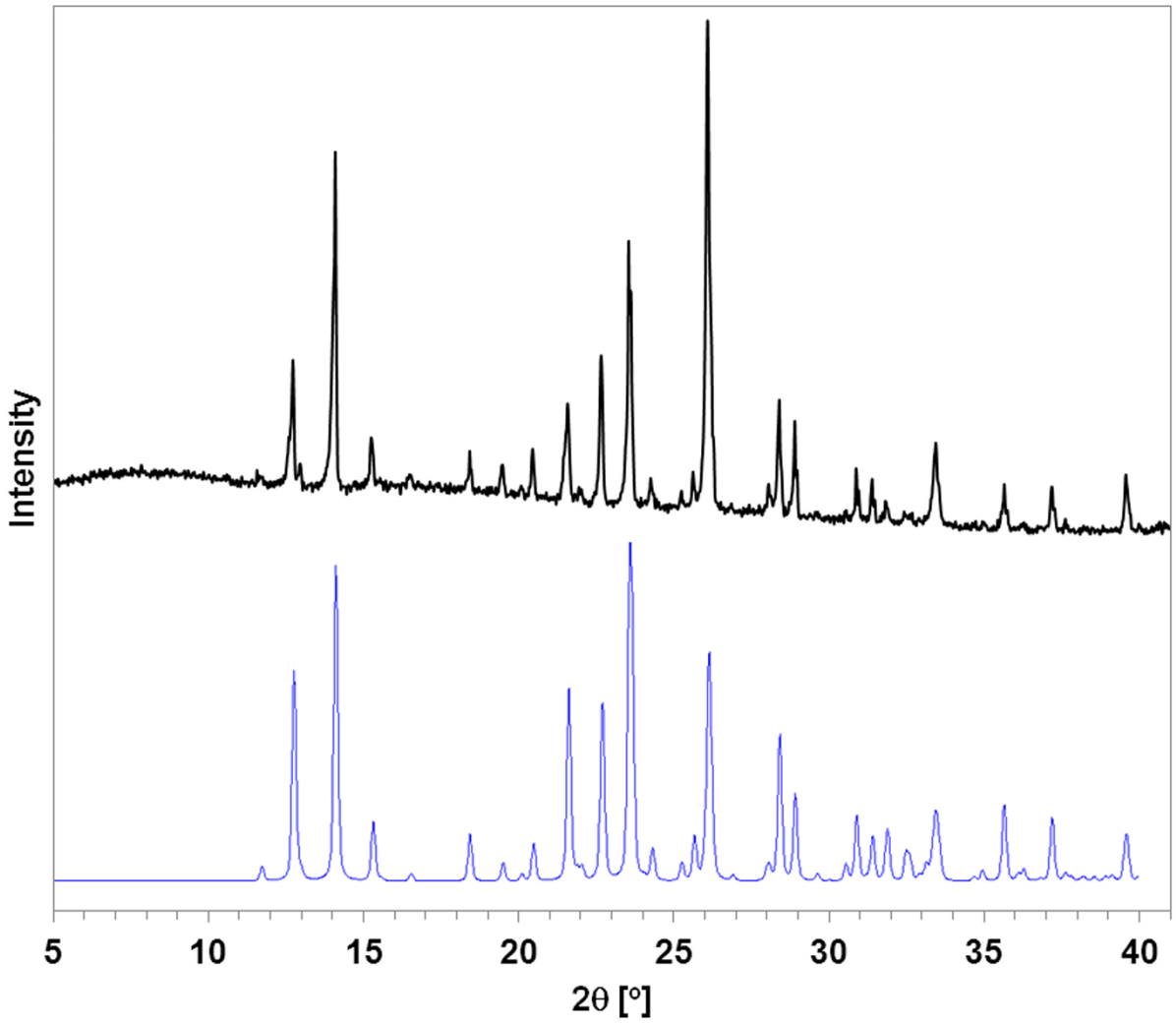


Fig. S1 Comparison of simulated (blue) and experimental (black) powder X-ray diffraction patterns for compound **1**.

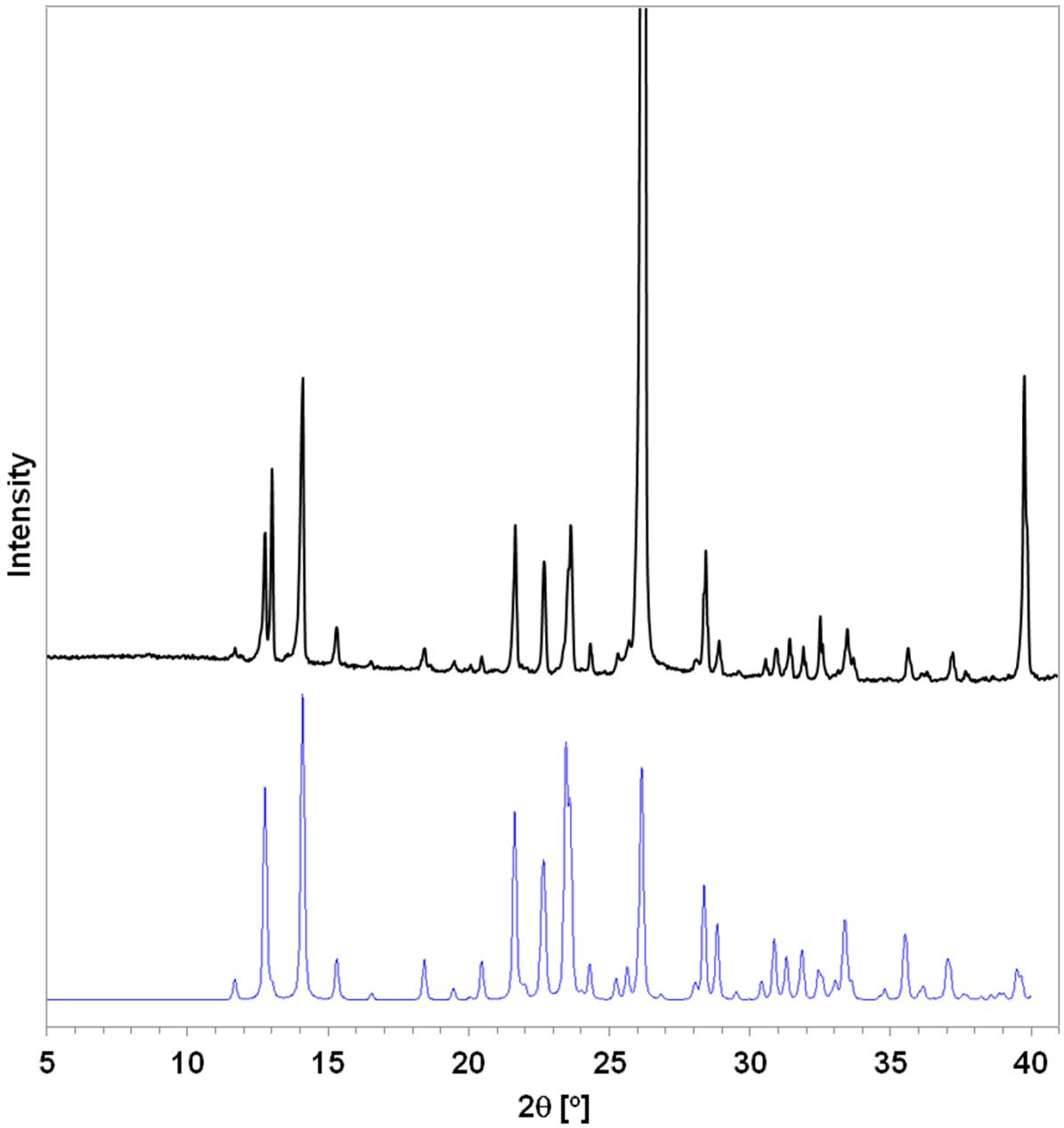


Fig. S2 Comparison of simulated (blue) and experimental (black) powder X-ray diffraction patterns for compound **2**.

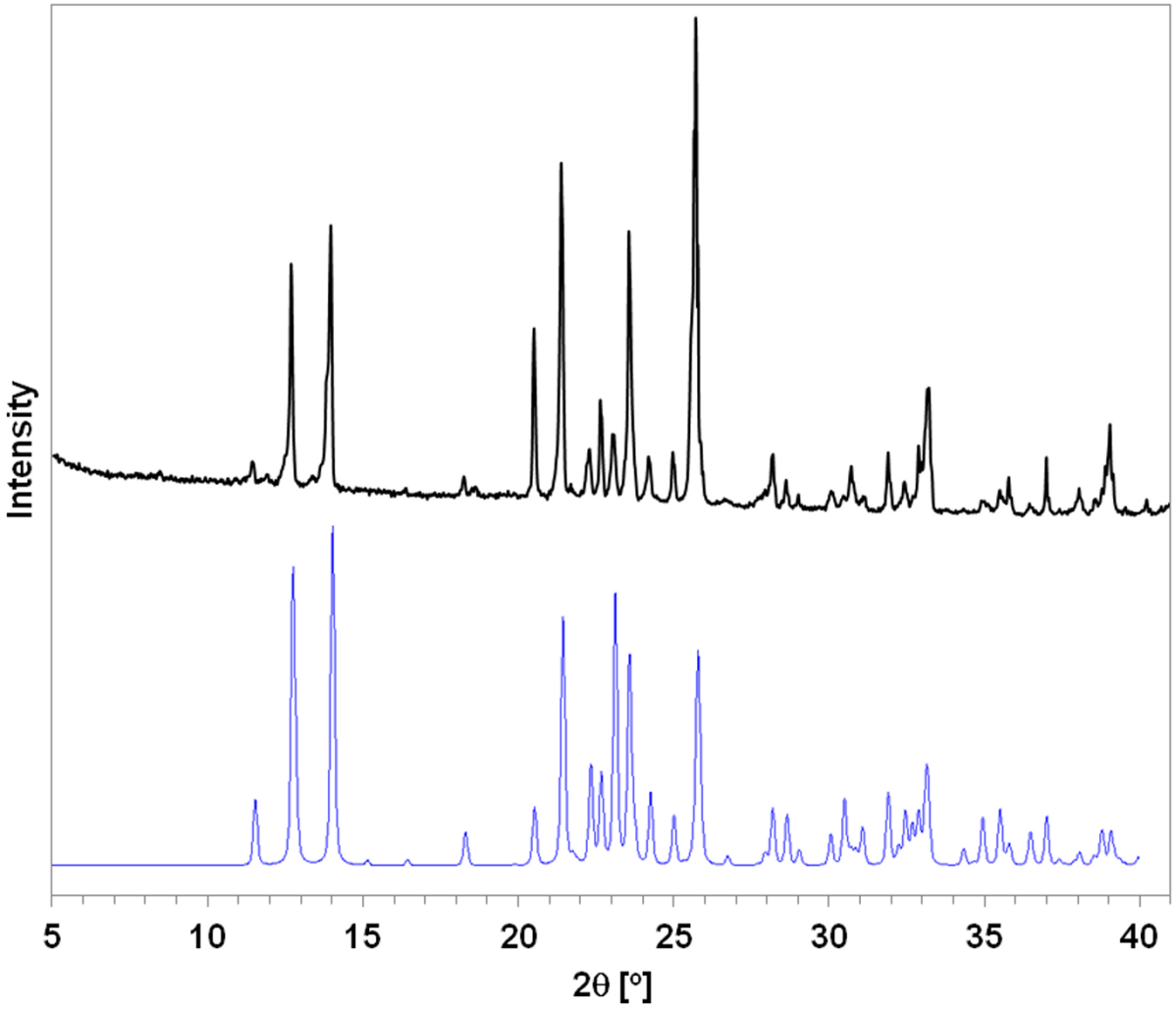
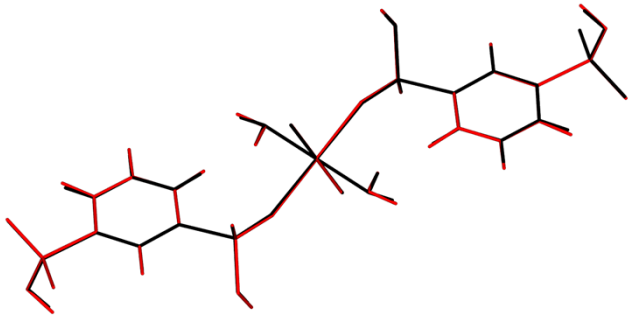
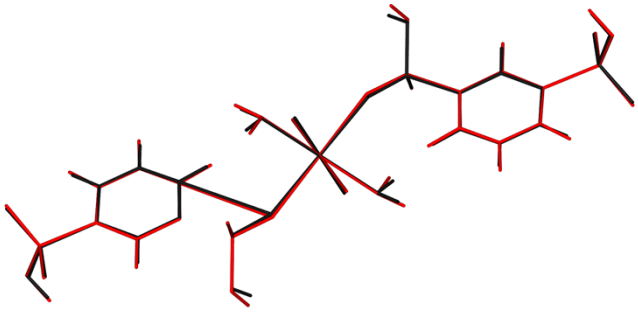


Fig. S3 Comparison of simulated (blue) and experimental (black) powder X-ray diffraction patterns for compound **3**.



(a)



(b)

Fig. S4 Superposition of experimental (black) and optimized (red) crystal structures of (a) compound **2** and (b) compound **3**.

Table S1. Atomic coordinates of the CRYSTAL09-optimized crystal structures of compounds **2** and **3**.

Compound **2**			
_atom_site_label			
_atom_site_fract_x			
_atom_site_fract_y			
_atom_site_fract_z			
Zn	4.332408683506E-20	1.954123817023E-20	-6.232825597122E-20
N1	-4.410267203522E-01	-2.720599899454E-01	3.957543450705E-02
H1N	-4.124265158421E-01	-2.725540079474E-01	1.301927562377E-01
C2	4.438644379696E-01	-1.877864370742E-01	-6.101449985409E-03
H2	3.854905505968E-01	-1.219902672604E-01	5.314556097468E-02
C3	4.043909151838E-01	-1.896093103949E-01	-1.242710258555E-01
C4	4.864535969819E-01	-2.800592920214E-01	-1.936556197137E-01
H4	4.567495122965E-01	-2.839494902111E-01	-2.862371620308E-01
C5	-3.959963847251E-01	-3.683510299890E-01	-1.438037959825E-01
C6	-3.613117476612E-01	-3.601439522617E-01	-2.476254394744E-02

H6	-2.720208355151E-01	-4.223318129272E-01	2.290468637859E-02
P3	2.378295413949E-01	-9.253764748301E-02	-1.858912445329E-01
O31	1.858607876604E-01	1.405483555158E-02	-9.573526060195E-02
O32	1.344300924989E-01	-2.224820571995E-01	-2.348945995807E-01
O33	2.843390714034E-01	-3.013990655242E-03	-2.963014113052E-01
H33	3.217601828755E-01	1.058126379470E-01	-2.823323541745E-01
P5	-2.854254841208E-01	-4.912152015570E-01	-2.288139927004E-01
O51	-3.632401696717E-01	4.922429813333E-01	-3.495134896775E-01
O52	-2.481962163670E-01	3.614219749906E-01	-1.599292973609E-01
O53	-1.365681166469E-01	-3.912036780688E-01	-2.298634383058E-01
H53	-1.633074100476E-01	-2.900896207057E-01	-2.676030796622E-01
O1W	1.249044055075E-02	-2.470078818525E-01	4.454789046810E-03
H1W	9.597780421422E-02	-2.951030979700E-01	5.119606593153E-02
H2W	7.469585224542E-04	-2.940077007345E-01	-7.168725091952E-02

Compound **3**

_atom_site_label			
_atom_site_fract_x			
_atom_site_fract_y			
_atom_site_fract_z			
Cd	-1.444112965012E-19	9.524493683410E-36	0.000000000000E+00
N1	-4.471837554199E-01	-2.671463096121E-01	3.780834530831E-02
H1N	-4.198937266959E-01	-2.682918406008E-01	1.273567623385E-01
C2	4.383895704929E-01	-1.864705991800E-01	-1.015751038690E-02
H2	3.756215648089E-01	-1.237976479857E-01	4.670576609137E-02
C3	4.052765438539E-01	-1.877007104685E-01	-1.278395424496E-01
C4	4.920881396231E-01	-2.748875636434E-01	-1.938782945539E-01
H4	4.674241958657E-01	-2.774542106350E-01	-2.858196287446E-01
C5	-3.917019898998E-01	-3.600501941246E-01	-1.415134888776E-01
C6	-3.626619221309E-01	-3.515643204717E-01	-2.342733606211E-02
H6	-2.740429876680E-01	-4.105093092502E-01	2.574019055614E-02
P3	2.439370229019E-01	-8.895670159000E-02	-1.934590464751E-01
O31	1.947180528868E-01	2.293104676910E-02	-1.066632846133E-01
O32	1.389277707409E-01	-2.167382842538E-01	-2.405400089238E-01

O33	2.944312718635E-01	-1.380728857990E-03	-3.019855176344E-01
H33	3.253455535691E-01	1.091872150013E-01	-2.862602543827E-01
P5	-2.762149256123E-01	-4.814798420827E-01	-2.208568899798E-01
O51	-3.423541388047E-01	-4.972417453580E-01	-3.429590799996E-01
O52	-2.441145837206E-01	3.704004141418E-01	-1.530010818435E-01
O53	-1.291308796969E-01	-3.793838601507E-01	-2.163254109629E-01
H53	-1.527112884529E-01	-2.814664618759E-01	-2.576349530474E-01
O1W	1.229805083469E-02	-2.727308684746E-01	3.907574287393E-03
H1W	9.668026166576E-02	-3.184956236083E-01	4.916269694686E-02
H2W	-5.268683180690E-03	-3.244609373693E-01	-6.949857680709E-02

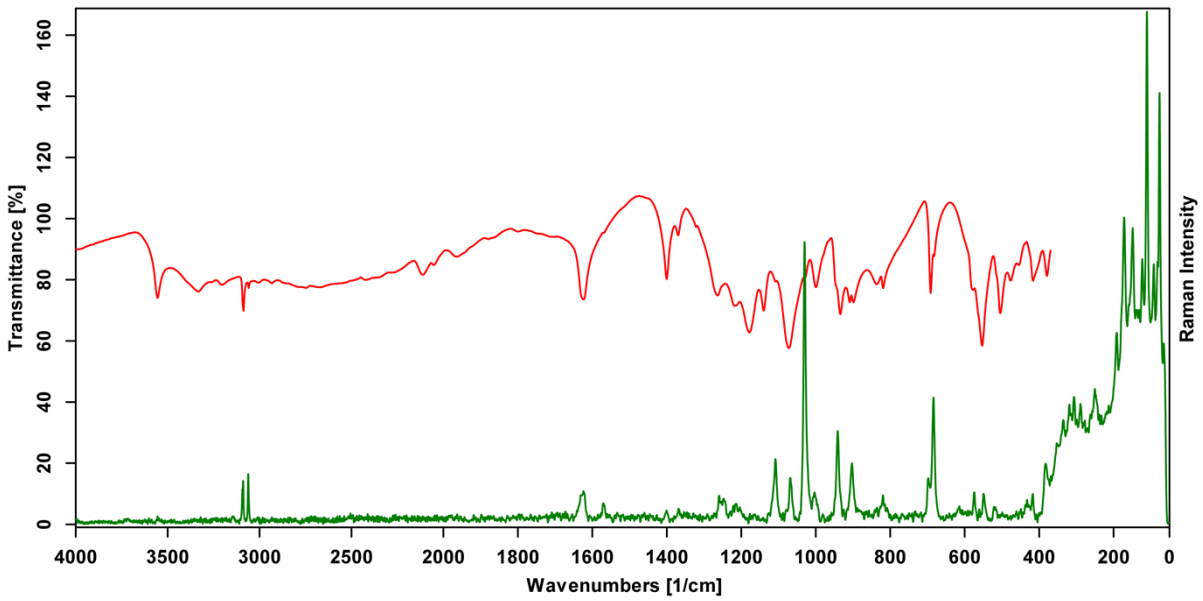


Fig. S5 Complementary IR (red) and Raman (green) spectra of compound **1**.

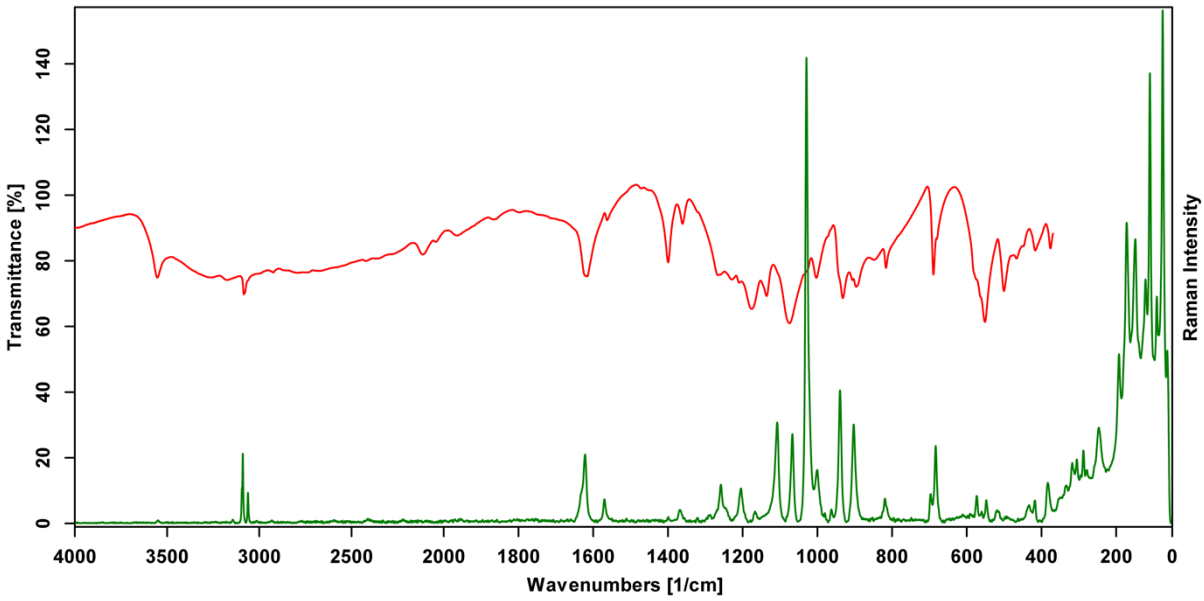


Fig. S6 Complementary IR (red) and Raman (green) spectra of compound **2**.

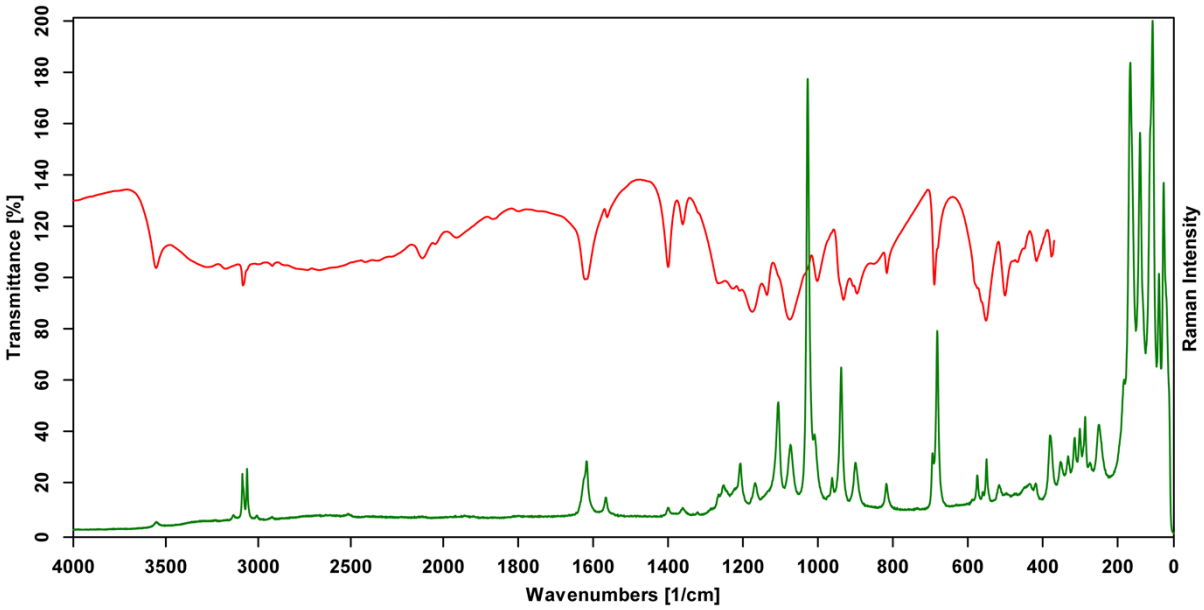


Fig. S7 Complementary IR (red) and Raman (green) spectra of compound **3**.

Table S2 Positions and assignments of vibrational bands, observed in FTIR and Raman spectra of compounds **1**-**3**.

1		**2**		**3**		
IR	Raman	IR	Raman	IR	Raman	Band assignment[a)]
3555 s		3553 s		3553 s		$\nu(O–H)_{water}$
3333 s br		3265 s br		3276 s br		ν(N–H)
3261 m		3176 s		3178 s		
3204 m						
3087 s	3089 vw	3084 s	3089 vw	3083 s	3086 vw	ν(C–H)
3059 m	3062 vw		3061 vw		3061 vw	
3005 m				3004 m		
2933 m		2925 s		2925 m		
2853 m br		2854 s br		2854 m br		ν(O–H)
		2795 s br				
2747 m br		2746 s br		2735 s br		
2676 m br		2672 s br		2668 s br		
2422 m br		2422 m br		2422 m br		
2355 m br		2362 m br		2358 m br		
2283 m br		2284 m br		2283 m br		
2113 m		2114 m		2113 m		
2052 m		2044 m		2044 m		
1964 w		1965 w		1965 m		
1880 w		1868 w		1868 w		
1800 w		1797 vw		1800 w		
1624 s	1624 vw	1616 s	1622 vw	1622 s	1618 vw	ν(C=C)
	1570 vw	1562 w	1570 vw	1562 w	1566 vw	
1400 m		1399 m		1399 s	1400 vw	ν(C=N)
1369 w		1361 w		1361 w	1361 vw	
1263 s	1260 vw	1266 s	1258 vw	1266 s	1251 vw	δ(N–H)
1218 s		1230 s		1227 s		
	1204 vw	1209 s	1204 vw	1209 s	1207 vw	
1178 vs		1176 vs		1176 vs		ν(P=O)

					1168 vw	
1140 s		1136 s		1136 vs		
	1108 vw		1108 vw		1106 w	
1072 vs	1068 vw	1075 vs	1067 vw	1075 vs	1073 vw	ν(P–O)
	1030 m		1029 vs		1027 vs	δ(C–H)
999 m	1003 vw	1003 s	1000 vw	1002 s	1009 vw	ν(P–C)
					962 vw	
933 s	941 vw	932 vs	939 w	932 vs	938 w	ν(P–O)
909 s						
	903 vw		903 vw		900 vw	
899 s		896 s		896 s		
836 m		849 m		852 m		γ(C–H)
819 m	820 vw	817 m	819 vw	816 s	817 vw	
	698 vw		697 vw		694 vw	
691 s	684 w	690 s	683 vw	690 s	681 w	out-of-plane ring def. vib.
	574 vw		573 vw		575 vw	
553 vs	549 vw	552 vs	548 vw	552 vs	550 vw	δ(PO_2)
					516 vw	
504 s		500 s		500 vs		
476 m		467 m		468 m		
					435 vw	
417 m	417 vw	417 m	418 vw	417 m	419 vw	
379 m	383 vw	376 m	383 vw	377 m	380 vw	
	353 vw				353 vw	
	335 vw		334 vw		332 vw	
	319 w		318 vw		314 vw	
	306 w		306 vw		301 vw	
	289 w		288 vw		287 w	
	277 vw		278 vw		274 vw	
	250 w		247 vw		250 w	
	192 w		193 w			
					183 w	

172 m	172 m	
		166 vs
149 m	149 m	
		140 s
123 m	122 m	
111 vs	110 vs	107 vs
92 m	91 m	90 m
77 vs	76 vs	77 s
65 w	64 w	

[a)]Abbreviations: vs – very strong, s – strong, m – medium, w – weak, vw – very weak, br – broad, ν – stretching, δ – in-plane deformation vibration, γ – out-of-plane deformation vibration.

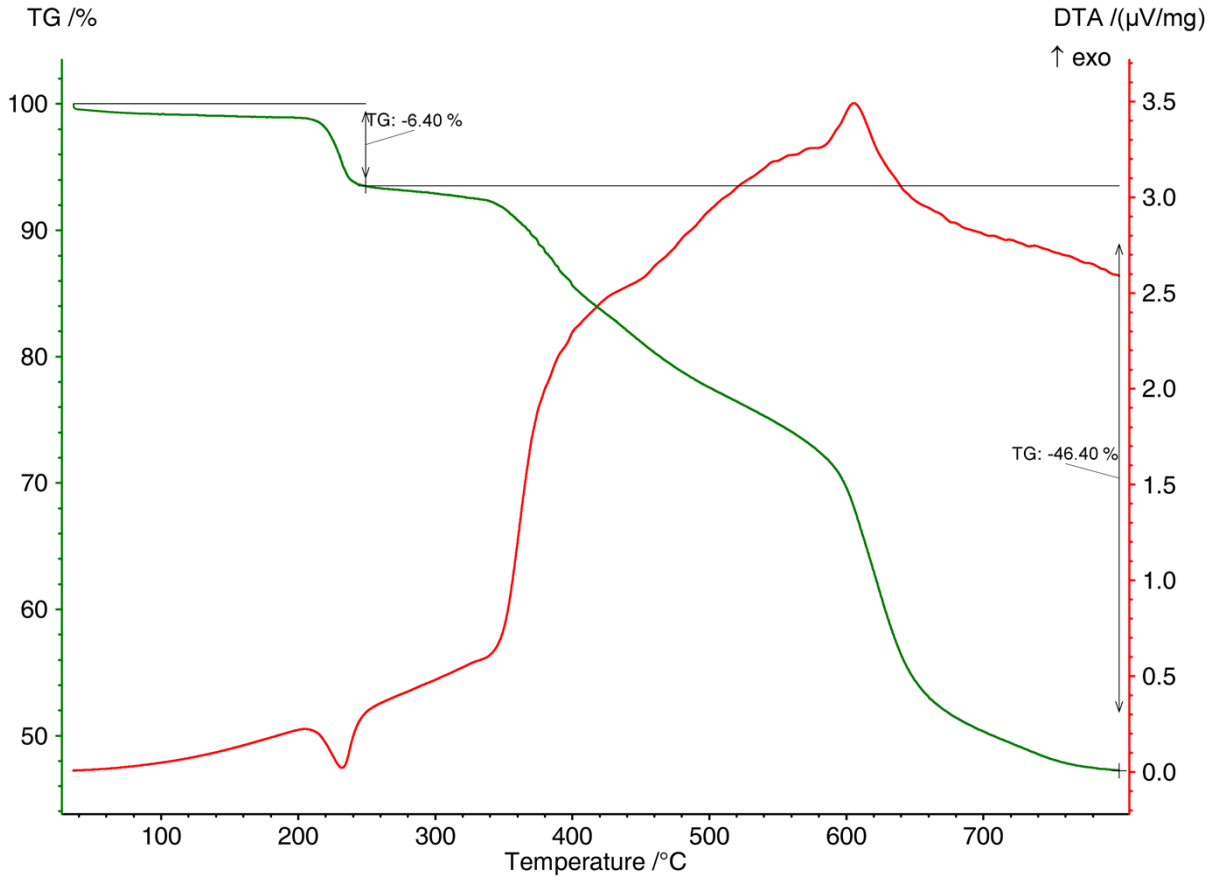


Fig. S8 TG-DTA curves of compound **1**.

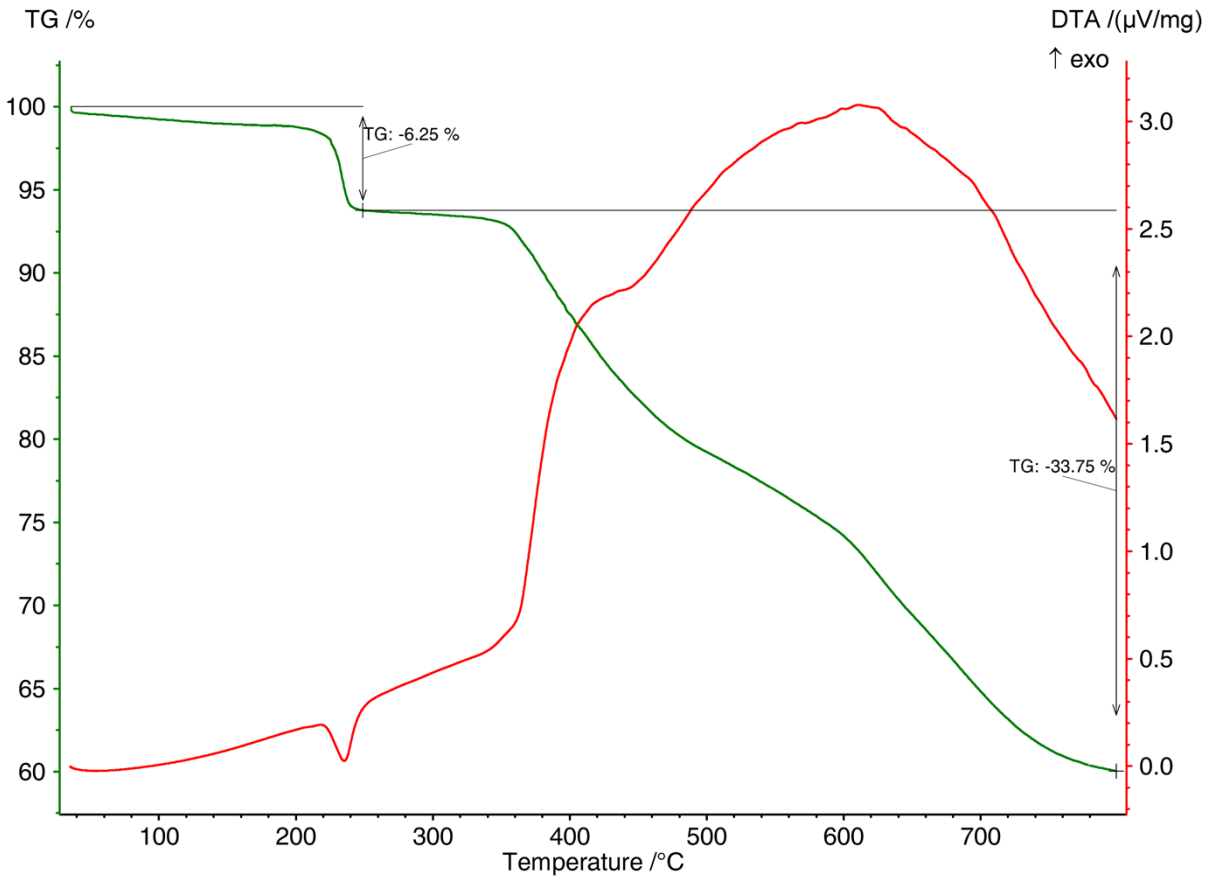


Fig. S9 TG-DTA curves of compound **2**.

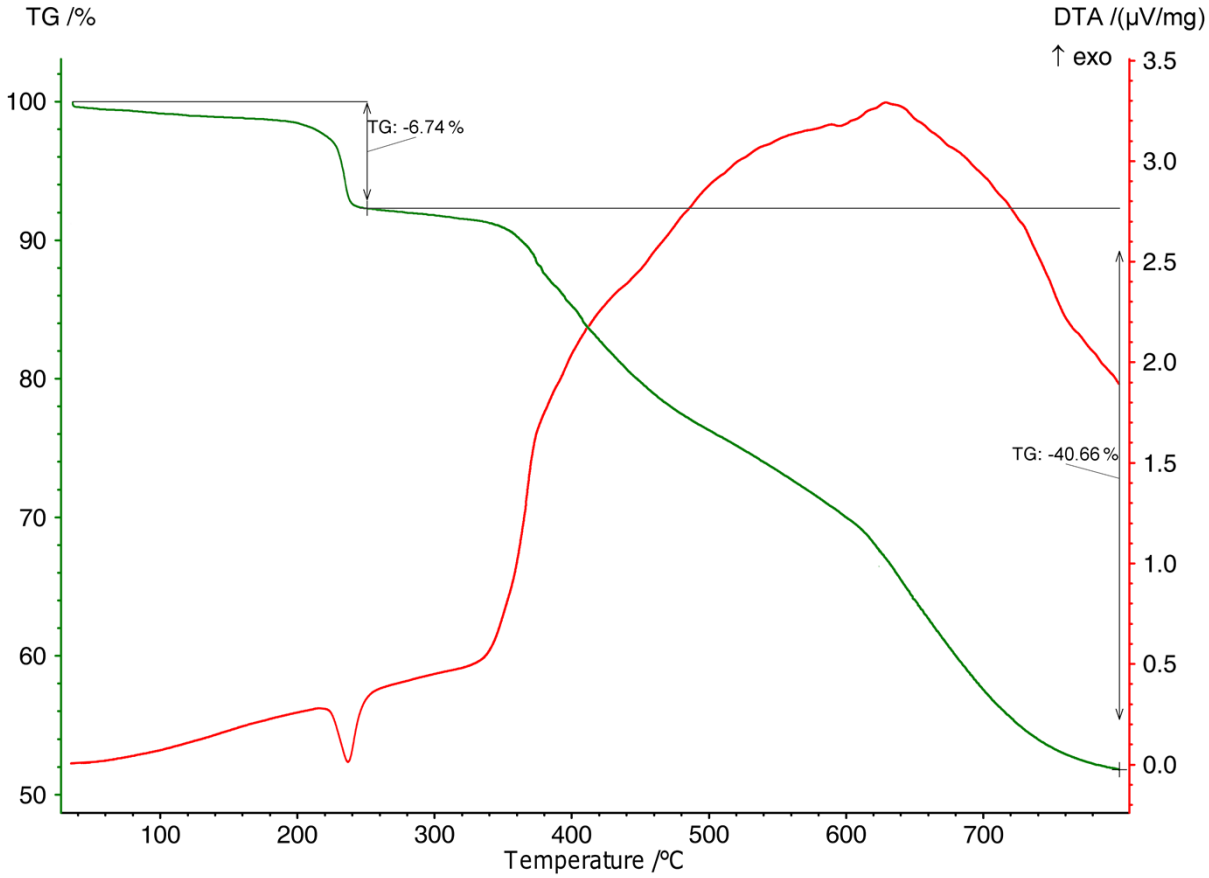


Fig. S10 TG-DTA curves of compound **3**.