STRUCTURAL CHEMISTRY

Volume 73 (2017)

Supporting information for article:

Synthesis, structural characterization and computational studies of *catena*-poly[chlorido[μ3-(pyridin-1-ium-3-yl)phosphonato-$\kappa^3O:O':O''$]zinc(II)]

Magdalena Wilk-Kozubek, Katarzyna N. Jarzembska, Jan Janczak and Veneta Videnova-Adrabinska

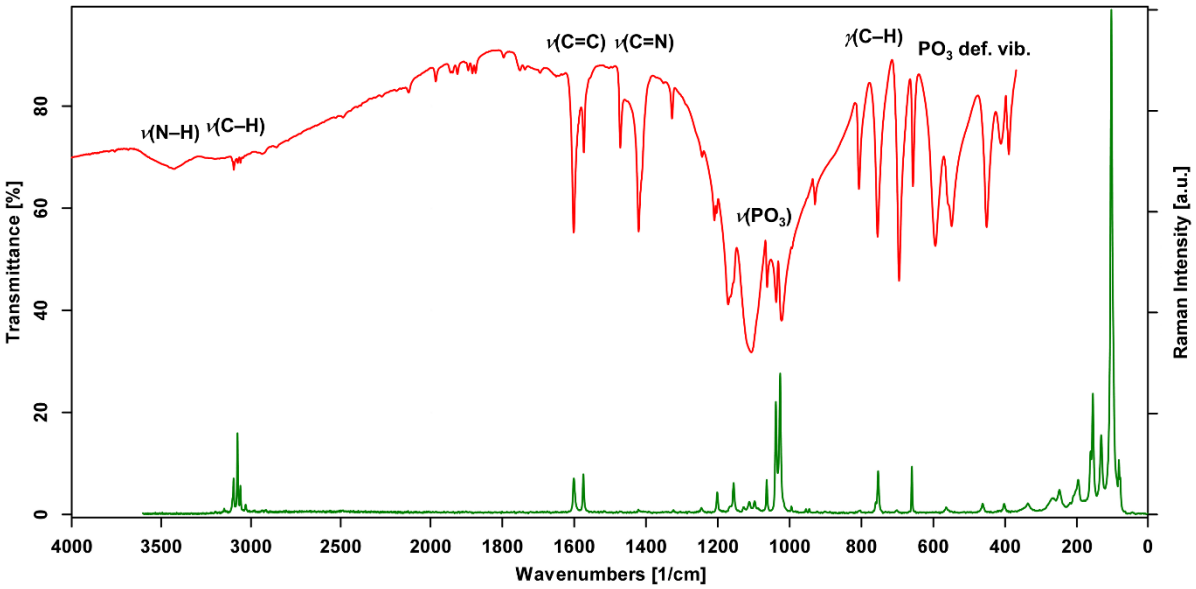

Figure S1 The complementary FT-IR (upper) and FT-Raman (lower) spectra of compound (1).

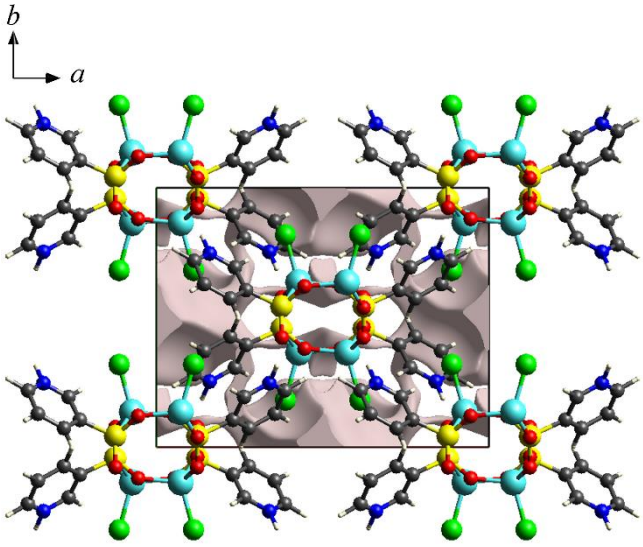

Figure S2 The void surface (0.002 au) for a unit cell of compound (1).

Table S1 Positions and assignments of vibrational bands, observed in FT-IR and FT-Raman spectra of compound (1)

IR	Raman	Band asgmt[a]	IR	Raman	Band asgmt[a]
3427 w		ν(N–H)	1244 w		
3200 w			1209 m	1202 vw	δ(C–H)
3096 w	3097 vw	ν(C–H)	1172 vs		δ(N–H)
3073 w	3075 vw			1156 vw	δ(C–H)
3059 w	3059 vw		1107 vs		$\nu_{as}(PO_3)$
2937 w			1063 s	1064 vw	δ(C–H)
2858 w			1038 vs	1038 w	
2487 w			1023 vs	1026 w	$\nu_{s}(PO_3)$
2122 vw			930 m		
1986 vw			807 m		γ(C–H)
1938 vw			755 s	754 vw	
1925 vw			695 s		ring def. vib.
1895 vw			657 m	660 vw	
1883 vw			594 s		PO_3 def. vib.
1875 vw			549 m		
1797 vw			451 m		
1751 vw			412 w		
1737 vw			390 w		
1694 vw				249 vw	
1650 vw				197 vw	
1602 m	1601 vw	ν(C=C)		156 w	
1573 w	1575 vw			133 vw	
1472 w		ν(C=N)		104 vs	
1420 m				83 vw	
1328 w					

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