

Table S1. The comparison of the theoretical and experimental wavenumber for the IP6Cu.

Calc. wavenumber	Relative intensity%*	IR exp.	RS exp.	Assignment
3743	5	3348sh		$\nu(\text{H}_2\text{O})$
3741	4			
3732	6			
3710	8			
3392	16	3244w 3158sh		$\nu(\text{O-H}\cdots\text{O})$ intermolecular
3224	28			
3119	44			
3119	4			
2962	47	2944sh 2935m		$\nu(\text{CH})$
		2790s		$\nu(\text{A,B,C})$ – Fermi resonance
2399	46	2341m		
2346	100	2137sh		
		1770 sh 1688 sh 1629m	1788- 1791, 1600	$\delta(\text{H}_2\text{O})$
1466	7		1463	$\nu(\text{OH}\cdots\text{O})$
1315	1	1396w	1393- 1395	$\delta(\text{CH})$
1312	1			
			1274- 1278	+ $\nu_{\text{as}}(\text{PO}_4)$
1300	4	1212w		$\delta(\text{OH}\cdots\text{O})$
1292	3			
1259	6			
1230	5			
1192	7	1153sh		$\nu(\varphi) + \delta(\text{CH})$
1151	4			
1137	3			
1122	5	1116m		$\nu_{\text{as}}(\text{PO}_4)$
1117	6			
1106	4			
1102	6	1046m	1066- 1069	$\nu(\text{C-O}) + \nu_{\text{as}}(\text{PO}_4)$
1096	28			
1075	9			
1057	5	1039sh 937vs		$\nu_{\text{as}}(\text{PO}_4)$
1052	1			
1045	18			
1028	4			
1023	7			
1018	4	902sh	902-905	$\nu_{\text{s}}(\text{PO}_4)$
1015	20			
1010	2			
1005	5			
1000	1			

993	2			
986	4	889sh		$\gamma(\text{CH})$
941	3			
931	4			
908	12			
903	3			
880	3			
872	9	859sh	859-860	$\gamma(\text{OH}) + \gamma(\text{O-H}\cdots) + \nu_s(\text{PO}_4)$
864	3			
842	12			
836	8			
816	7			
810	3	802sh	810-815	$\nu(\varphi)$ ring breathing + $\delta(\text{C-O-P})$
799	14			
793	4			
786	2			
779	2			
762	4	707m 668m	634-640	$\gamma(\text{OH}) + \nu(\text{PO}_4)$
749	2			
735	8			
729	8			
728	4			
708	4	632sh 614w		$\gamma(\varphi)$
671	2			
655	4			
632	2	580w 553sh		$\delta(\text{C-O-P})$
629	5			
608	1			
537	1	488m 454m	503-506	$\delta_{\text{as}}(\text{PO}_4)$
525	1			
498	2			
471	1			
459	2			
441	2	418w	401-403	$\delta_s(\text{PO}_4) + \nu(\text{CuO})$
421	3			
418	3			
409	2			
402	1			
390	2			
383	4			
381	2			
368	1			
360	3		260-264	$\nu(\text{CuO}) + \nu(\text{O}\cdots\text{H})$
337	6			
318	4			
284	1			
278	1			
275	1			

248	1			
232	4			
197	1			
195	2			
186	1			
180	1	150	143	$\nu(\text{O}\cdots\text{H}) + \nu(\text{CuO}_6)$
106	1			

abbreviations used: s, strong; m, medium; w, weak; v, very; sh, shoulder; ν , stretching (s, symmetric; as, asymmetric); δ , scissoring; and ϕ , inositol ring;

* In the comparison of the theoretical and experimental wavenumber for the IP6Cu modes having intensity greater than 1%.