Supplemental Material

Table S1. The powder pattern of monoclinic $FePO_4$

h	k	l	$2\theta_{obs}$	$2\theta_{cacl}$	d_{hkl} (Å)	Intensity
0	1	1	7.424	7.430	5.4781	77
1	0	-1	8.592	8.579	4.7345	100
1	1	0	9.224	9.219	4.4108	46
1	0	1	9.427	9.431	4.3160	17
1	1	-1	10.165	10.156	4.0034	94
1	1	1	10.885	10.886	3.7393	38
0	1	2	11.510	11.521	3.5369	53
0	2	1	11.998	11.996	3.3935	43
1	1	-2	13.172	13.159	3.0922	22
1	2	1	14.377	14.405	2.8342	67
0	2	2	14.889	14.892	2.7373	39
2	1	0	15.894	15.892	2.5651	29
1	2	-2	16.204	16.197	2.5163	14
2	1	1	17.147	17.150	2.3789	15
1	0	3	17.668	17.669	2.3093	7
2	1	-2	18.043	18.054	2.2617	9
1	3	-1	18.465	18.469	2.2104	13
2	2	-1	18.781	18.782	2.1736	21
1	3	2	21.060	21.052	1.9406	28
0	4	0	21.825	21.825	1.8734	7
3	0	-1	22.497	22.534	1.8181	4
2	1	3	23.136	23.140	1.7686	25
3	0	1	23.627	23.556	1.7323	10
2	0	-4	24.095	24.091	1.6991	6
3	2	-1	25.054	25.078	1.6351	16
3	0	-3	25.954	25.934	1.5793	9
3	1	2	26.286	26.240	1.5597	16
1	3	-4	26.718	26.718	1.5349	24
1	0	5	27.387	27.398	1.4981	5
2	4	-2	27.920	27.925	1.4701	37
3	0	3	28.514	28.556	1.4401	8
2	1	-5	28.896	28.897	1.4215	10
0	4	4	30.043	30.043	1.3684	7
4	1	0	30.588	30.621	1.3445	14
2	5	-1	31.498	31.496	1.3066	12
4	0	2	32.855	32.854	1.2540	11
4	1	2	33.312	33.324	1.2373	8

Table S2. H-bond geometry in hydrates A and B.

Atoms D-H…A	δ(D-H)	δ(H…A)	δ(D...A)	DHA	Symm.
			Compound A		
O5-H51-O3	0.80(3)	2.41(5)	3.018(6)	135(6)	-x-1/2, y+1/2, -z+3/2
O5-H52-O2	0.80(3)	2.41(5)	3.044(6)	138(7)	-x, -y+1, -z+2
O5-H52-O4	0.80(3)	2.20(5)	2.847(6)	138(7)	-x, -y+1, -z+2
O5-H52-O3	0.80(3)	2.36(5)	3.070(6)	148(7)	-x+1/2, y+1/2, -z+3/2
O6-H61-O1	0.79(3)	1.91(4)	2.641(5)	152(7)	x+1, y, z
O6-H62-O2	0.80(3)	1.89(4)	2.617(5)	152(7)	
O6-H62-O4	0.80(3)	2.57(6)	3.102(5)	126(6)	x+1, y, z
			Compound B		
O5-H51-O6	0.794(10)	2.65(5)	3.043(2)	112(4)	-x+1, y+1/2, -z+1/2
O5-H52-O2	0.796(10)	1.863(15)	2.638(2)	164(4)	x+1/2, y, -z+1/2
O6-H61-O1	0.795(10)	1.885(12)	2.670(2)	169(4)	x, -y+1/2, z+1/2
O6-H61-O3	0.795(10)	2.61(4)	2.996(2)	112(3)	x, -y+1/2, z+1/2
O6-H62-O4	0.791(10)	1.904(19)	2.655(2)	158(5)	-x+1/2, y-1/2, z
O6-H62-O2	0.791(10)	2.59(4)	3.142(2)	128(4)	-x+1/2, y-1/2, z