SUPLEMENTARY MATERIAL

Figure S1. Observed (circles), calculated (solid line), and difference (at the bottom) D2B neutron diffraction profiles at room temperature (λ= 1.594Å) of (a) $Mo(PO_3)_3$ and (b) $Fe(PO_3)_3$. Vertical marks correspond to the position of the reflections.

Table S1. Final refined positional and thermal parameters from D2B neutron diffraction patterns (λ= 1.594Å) at room temperature for $Mo(PO_3)_3$.

Table S2. Main interatomic distances (Å) and angles (º) for $Mo(PO_3)_3$ at room temperature.

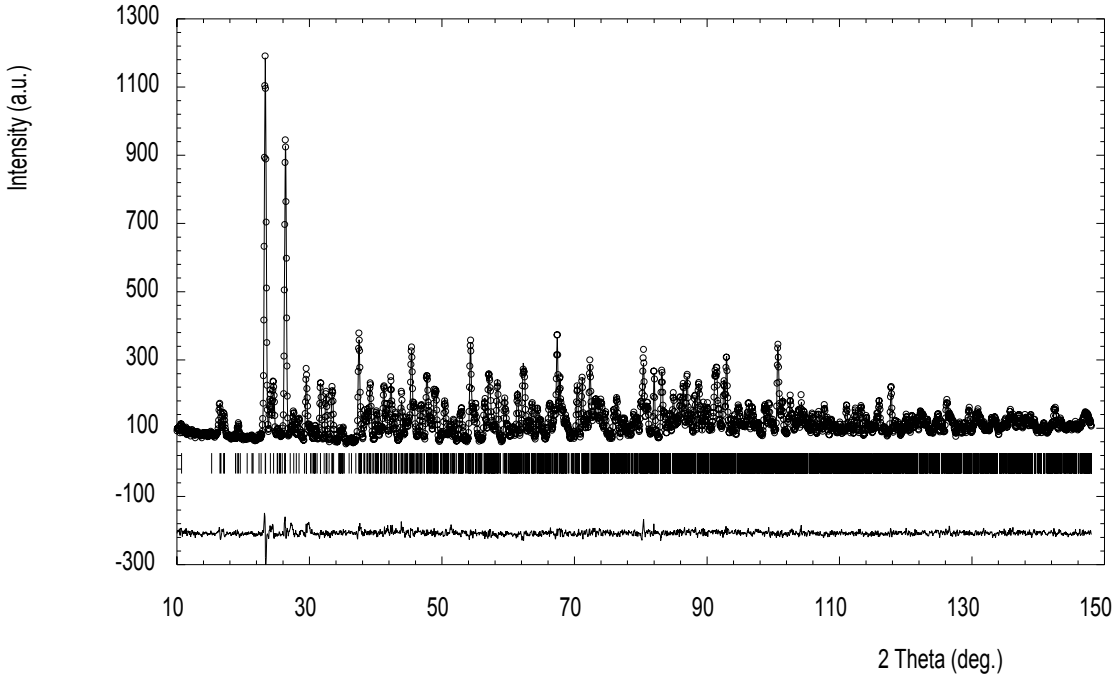

Fig S1(a)

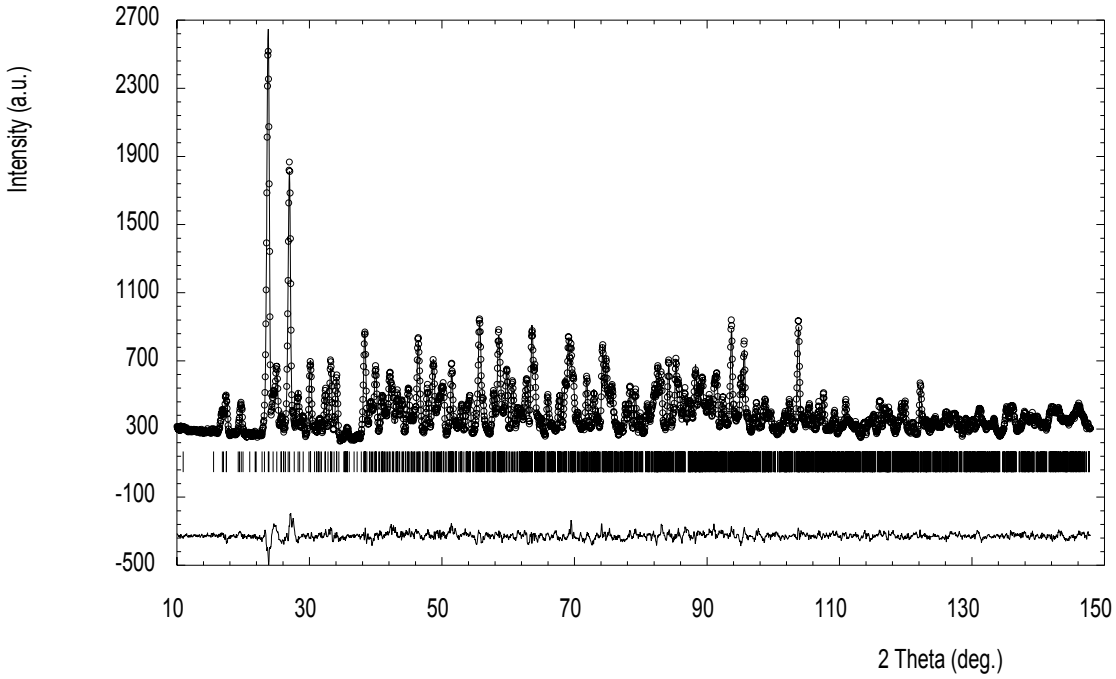

Figure S1(b)

Table S1. Final refined positional and thermal parameters from D2B neutron diffraction patterns (λ= 1.594Å) at room temperature for $Mo(PO_3)_3$.

Atom	x	y	z	B(Å^2)
Mo(1)	0	0.1687(9)	0	0.81(7)
Mo(2)	0.497(3)	0.1588(7)	0.007(3)	0.81(7)
Mo(3)	0.478(2)	-0.0054(7)	0.519(2)	0.81(7)
P(1)	0.136(2)	0.1116(9)	0.318(2)	0.59(5)
P(2)	0.342(3)	0.1112(9)	0.705(2)	0.59(5)
P(3)	0.135(3)	0.0516(9)	0.833(2)	0.59(5)
P(4)	0.723(3)	0.1090(9)	0.521(3)	0.59(5)
P(5)	0.349(2)	0.051(1)	0.200(3)	0.59(5)
P(6)	0.647(2)	0.222(1)	0.318(2)	0.59(5)
P(7)	0.858(3)	0.2195(9)	0.686(2)	0.59(5)
P(8)	0.261(2)	0.2288(8)	0.495(2)	0.59(5)
P(9)	0.749(2)	0.0587(9)	-0.000(2)	0.59(5)
O(1)	-0.114(3)	0.2525(9)	0.053(2)	0.98(3)
O(2)	-0.034(2)	0.1985(8)	-0.208(2)	0.98(3)
O(3)	-0.165(2)	0.1146(7)	-0.041(2)	0.98(3)
O(4)	0.095(2)	0.0840(8)	-0.038(2)	0.98(3)
O(5)	0.152(2)	0.2350(7)	0.028(2)	0.98(3)
O(6)	0.036(2)	0.1436(7)	0.214(2)	0.98(3)
O(7)	0.546(3)	0.2177(8)	0.190(2)	0.98(3)
O(8)	0.368(2)	0.2332(7)	-0.059(2)	0.98(3)
O(9)	0.628(2)	0.2186(7)	-0.093(2)	0.98(3)
O(10)	0.630(2)	0.0821(7)	0.048(2)	0.98(3)
O(11)	0.368(2)	0.1082(7)	0.100(2)	0.98(3)
O(12)	0.448(2)	0.1152(7)	-0.187(2)	0.98(3)
O(13)	0.625(2)	0.0630(7)	0.560(2)	0.98(3)
O(14)	0.441(2)	0.0396(7)	0.316(2)	0.98(3)
O(15)	0.524(2)	-0.0321(8)	0.729(2)	0.98(3)
O(16)	0.592(2)	-0.0819(7)	0.449(2)	0.98(3)
O(17)	0.355(2)	0.0624(7)	0.584(2)	0.98(3)
O(18)	0.337(2)	-0.0793(8)	0.474(2)	0.98(3)
O(19)	0.212(2)	0.0588(7)	0.246(2)	0.98(3)
O(20)	0.233(2)	0.1699(7)	0.374(2)	0.98(3)
O(21)	0.324(2)	0.1872(7)	0.631(2)	0.98(3)
O(22)	0.210(2)	0.1034(7)	0.762(2)	0.98(3)
O(23)	0.212(2)	-0.0138(8)	0.867(2)	0.98(3)
O(24)	0.660(2)	0.1546(7)	0.403(2)	0.98(3)
O(25)	0.757(2)	0.1599(8)	0.650(2)	0.98(3)
O(26)	0.329(2)	-0.0183(7)	0.126(2)	0.98(3)
O(27)	0.773(3)	0.2721(9)	0.760(2)	0.98(3)

Table S2. Main interatomic distances (Å) and angles (º) for $Mo(PO_3)_3$ at room temperature.

$Mo(PO_3)_3$					
Bond Distances Mo-O (Å)					
Mo(1)-(O1)	2.15(2)	Mo(2)-(O7)	2.10(3)	Mo(3)-(O13)	2.06(2)
Mo(1)-(O2)	2.06(2)	Mo(2)-(O8)	2.05(3)	Mo(3)-(O14)	2.12(2)
Mo(1)-(O3)	2.06(2)	Mo(2)-(O9)	2.15(3)	Mo(3)-(O15)	2.08(3)
Mo(1)-(O4)	2.00(2)	Mo(2)-(O10)	2.06(2)	Mo(3)-(O16)	2.10(2)
Mo(1)-(O5)	2.08(2)	Mo(2)-(O11)	2.01(3)	Mo(3)-(O17)	2.03(3)
Mo(1)-(O6)	2.09(2)	Mo(2)-(O12)	2.06(3)	Mo(3)-(O18)	2.10(3)
Bond Angles O-Mo-O (º)					
O(1)-Mo(1)-(O2)	89.0(1)	O(7)-Mo(2)-(O8)	87.5(1)	O(13)-Mo(3)-(O14)	87.3(1)
O(1)-Mo(1)-(O3)	85.6(1)	O(7)-Mo(2)-(O9)	88.4(1)	O(13)-Mo(3)-(O15)	84.1(1)
O(1)-Mo(1)-(O4)	173.9(1)	O(7)-Mo(2)-(O10)	98.4(1)	O(13)-Mo(3)-(O16)	92.9(1)
O(1)-Mo(1)-(O5)	88.0(1)	O(7)-Mo(2)-(O11)	90.4(1)	O(13)-Mo(3)-(O17)	92.1(1)
O(1)-Mo(1)-(O6)	88.9(1)	O(7)-Mo(2)-(O12)	171.2(2)	O(13)-Mo(3)-(O18)	176.6(2)
O(2)-Mo(1)-(O3)	85.3(1)	O(8)-Mo(2)-(O9)	86.4(1)	O(14)-Mo(3)-(O15)	169.7(2)
O(2)-Mo(1)-(O4)	94.7(1)	O(8)-Mo(2)-(O10)	172.9(1)	O(14)-Mo(3)-(O16)	92.7(1)
O(2)-Mo(1)-(O5)	89.5(1)	O(8)-Mo(2)-(O11)	89.9(1)	O(14)-Mo(3)-(O17)	87.8(1)
O(2)-Mo(1)-(O6)	177.1(2)	O(8)-Mo(2)-(O12)	85.7(1)	O(14)-Mo(3)-(O18)	93.2(1)
O(3)-Mo(1)-(O4)	89.9(1)	O(9)-Mo(2)-(O10)	89.9(1)	O(15)-Mo(3)-(O16)	93.4(1)
O(3)-Mo(1)-(O5)	171.8(2)	O(9)-Mo(2)-(O11)	176.3(2)	O(15)-Mo(3)-(O17)	86.6(1)
O(3)-Mo(1)-(O6)	96.4(1)	O(9)-Mo(2)-(O12)	85.4(1)	O(15)-Mo(3)-(O18)	95.5(1)
O(4)-Mo(1)-(O5)	96.7(1)	O(10)-Mo(2)-(O11)	93.6(1)	O(16)-Mo(3)-(O17)	174.8(2)
O(4)-Mo(1)-(O6)	87.4(1)	O(10)-Mo(2)-(O12)	87.8(1)	O(16)-Mo(3)-(O18)	83.7(1)
O(5)-Mo(1)-(O6)	88.4(1)	O(11)-Mo(2)-(O12)	95.2(1)	O(17)-Mo(3)-(O18)	91.1(1)
Bond Distances P-O (Å)					
P(1)-O(6)	1.50(3)	P(2)-O(12)	1.43(3)	P(3)-O(4)	1.49(3)
P(1)-O(16)	1.51(3)	P(2)-O(17)	1.51(2)	P(3)-O(15)	1.50(3)
P(1)-O(19)	1.53(3)	P(2)-O(21)	1.64(2)	P(3)-O(22)	1.51(3)
P(1)-O(20)	1.59(3)	P(2)-O(22)	1.60(3)	P(3)-O(23)	1.53(2)
P(4)-O(13)	1.47(3)	P(5)-O(11)	1.49(3)	P(6)-O(7)	1.53(3)
P(4)-O(18)	1.48(3)	P(5)-O(14)	1.41(3)	P(6)-O(9)	1.45(2)
P(4)-O(24)	1.52(3)	P(5)-O(19)	1.60(3)	P(6)-O(24)	1.55(2)
P(4)-O(25)	1.58(3)	P(5)-O(26)	1.54(2)	P(6)-O(27)	1.54(4)
P(7)-O(1)	1.44(3)	P(8)-O(5)	1.44(3)	P(9)-O(3)	1.50(2)
P(7)-O(2)	1.48(3)	P(8)-O(8)	1.52(3)	P(9)-O(10)	1.50(3)
P(7)-O(25)	1.60(3)	P(8)-O(20)	1.62(2)	P(9)-O(23)	1.54(3)
P(7)-O(27)	1.60(3)	P(8)-O(21)	1.60(3)	P(9)-O(26)	1.60(3)
Bond Angles O-P-O (º)					
O(6)-P(1)-O(16)	115.8(2)	O(12)-P(2)-O(17)	115.9(2)	O(4)-P(3)-O(15)	111.2(2)
O(6)-P(1)-O(19)	111.1(2)	O(12)-P(2)-O(21)	107.3(2)	O(4)-P(3)-O(22)	108.6(2)
O(6)-P(1)-O(20)	108.2(2)	O(12)-P(2)-O(22)	115.0(3)	O(4)-P(3)-O(23)	112.6(2)
O(16)-P(1)-O(19)	110.9(2)	O(17)-P(2)-O(21)	104.7(1)	O(15)-P(3)-O(22)	107.1(2)
O(16)-P(1)-O(20)	104.7(2)	O(17)-P(2)-O(22)	112.0(2)	O(15)-P(3)-O(23)	107.1(2)
O(17)-P(1)-O(20)	105.0(2)	O(21)-P(2)-O(22)	99.7(2)	O(22)-P(3)-O(23)	109.8(2)
O(13)-P(4)-O(18)	119.7(3)	O(11)-P(5)-O(14)	119.0(2)	O(7)-P(6)-O(9)	112.1(2)
O(13)-P(4)-O(24)	105.9(2)	O(11)-P(5)-O(19)	109.3(2)	O(7)-P(6)-O(24)	111.8(2)
O(13)-P(4)-O(25)	106.3(2)	O(11)-P(5)-O(26)	112.0(1)	O(7)-P(6)-O(27)	106.6(3)
O(18)-P(4)-O(24)	107.7(2)	O(14)-P(5)-O(19)	111.9(3)	O(9)-P(6)-O(24)	111.6(2)
O(18)-P(4)-O(25)	111.5(2)	O(14)-P(5)-O(26)	104.6(3)	O(9)-P(6)-O(27)	111.0(2)
O(24)-P(4)-O(25)	104.2(2)	O(19)-P(5)-O(26)	97.5(2)	O(24)-P(6)-O(27)	102.9(2)
O(1)-P(7)-O(2)	118.2(3)	O(5)-P(8)-O(8)	121.1(3)	O(3)-P(9)-O(10)	116.0(2)
O(1)-P(7)-O(25)	107.1(2)	O(5)-P(8)-O(20)	115.0(2)	O(3)-P(9)-O(23)	107.3(2)
O(1)-P(7)-O(27)	110.1(3)	O(5)-P(8)-O(21)	109.6(2)	O(3)-P(9)-O(26)	105.4(2)
O(2)-P(7)-O(25)	113.0(2)	O(8)-P(8)-O(20)	99.6(2)	O(10)-P(9)-O(23)	106.9(2)
O(2)-P(7)-O(27)	108.0(2)	O(8)-P(8)-O(21)	105.7(2)	O(10)-P(9)-O(26)	108.0(2)
O(25)-P(7)-O(27)	98.2(2)	O(20)-P(8)-O(21)	103.8(2)	O(23)-P(9)-O(26)	113.2(2)