

Electronic Supplementary Information for Dalton Transactions

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters of $AM(PO_4)_2$ (A=Sr, M=Ti, Sn; A=Ba, M=Sn).

atom	Site	x	y	z	U_{eq}^a
SrTi(PO ₄) ₂					
Sr1	4e	0	0.19462(7)	3/4	0.00904(17)
Ti1	4c	1/4	1/4	1.00000	0.00449(19)
P1	8f	0.14208(4)	0.73878(13)	0.75611(9)	0.00474(19)
O1	8f	0.16408(11)	0.9629(3)	0.8966(2)	0.0076(4)
O2	8f	0.14674(11)	0.4797(3)	0.8561(2)	0.0075(4)
O3	8f	0.21688(13)	0.7329(4)	0.6923(3)	0.0080(4)
O4	8f	0.04818(13)	0.7784(4)	0.6036(3)	0.0115(4)
SrSn(PO ₄) ₂					
Sr1	4e	1/2	0.30812(8)	1/4	0.00885(12)
Sn1	4c	1/4	1/4	0	0.00423(11)
P1	8f	0.35839(4)	0.76022(11)	0.24157(8)	0.00413(16)
O1	8f	0.34213(10)	0.5367(4)	0.1035(2)	0.0079(4)
O2	8f	0.35673(10)	0.0167(4)	0.1418(2)	0.0078(3)
O3	8f	0.44899(12)	0.7242(3)	0.3982(2)	0.0106(4)
O4	8f	0.27942(12)	0.7676(3)	0.2879(2)	0.0081(4)
BaSn(PO ₄) ₂					
Ba1	2a	0	1.00000	0	0.0114(4)
Sn1	2c	0	1.00000	1/2	0.0053(4)
P1	4i	0.12946(17)	1/2	0.29232(17)	0.0077(5)
O1	8j	0.0210(3)	0.7400(5)	0.3112(3)	0.0108(8)
O2	4i	0.2602(4)	1/2	0.4408(5)	0.0110(9)

O3	4i	0.1872(5)	1/2	0.1162(5)	0.0145(10)
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^a U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond distances (Å) and angles (°) of AM(PO₄)₂ (A=Sr, M=Ti, Sn; A=Ba, M=Sn).

SrTi(PO ₄) ₂					
Sr1—O4 ⁱ	2.620(2)	Sr1—O4 ^v	2.741(2)	Ti1—O3 ^{vi}	1.8710(19)
Sr1—O4 ⁱⁱ	2.620(2)	Sr1—O4 ^{iv}	2.741(2)	Ti1—O3 ⁱⁱ	1.8710(19)
Sr1—O2	2.6270(17)	P1—O4	1.504(2)	Ti1—O1 ^{vii}	1.9631(17)
Sr1—O2 ⁱⁱⁱ	2.6270(17)	P1—O3	1.5336(19)	Ti1—O1 ^v	1.9631(17)
Sr1—O1 ^{iv}	2.6998(17)	P1—O2	1.5506(18)	Ti1—O2	1.9749(17)
Sr1—O1 ^v	2.6998(17)	P1—O1	1.5522(18)	Ti1—O2 ^{viii}	1.9749(17)
O3 ^{vi} —Ti1—O3 ⁱⁱ	180.000(1)	O3 ⁱⁱ —Ti1—O2	88.39(8)	O2—Ti1—O2 ^{viii}	180.000(1)
O3 ^{vi} —Ti1—O1 ^{vii}	88.31(8)	O1 ^{vii} —Ti1—O2	93.73(7)	O4—P1—O3	114.23(11)
O3 ⁱⁱ —Ti1—O1 ^{vii}	91.69(8)	O1 ^v —Ti1—O2	86.27(7)	O4—P1—O2	110.00(11)
O3 ^{vi} —Ti1—O1 ^v	91.69(8)	O3 ^{vi} —Ti1—O2 ^{viii}	88.39(8)	O3—P1—O2	107.41(10)
O3 ⁱⁱ —Ti1—O1 ^v	88.31(8)	O3 ⁱⁱ —Ti1—O2 ^{viii}	91.61(8)	O4—P1—O1	108.76(11)
O1 ^{vii} —Ti1—O1 ^v	180.000	O1 ^{vii} —Ti1—O2 ^{viii}	86.27(7)	O3—P1—O1	107.63(10)
O3 ^{vi} —Ti1—O2	91.61(8)	O1 ^v —Ti1—O2 ^{viii}	93.73(7)	O2—P1—O1	108.65(10)
(i) -x, 1-y, 1-z; (ii) x, 1-y, 0.5+z; (iii) -x, y, 1.5-z; (iv) -x, -1+y, 1.5-z; (v) x, -1+y, z; (vi) 0.5-x, -0.5+y, 1.5-z; (vii) 0.5-x, 1.5-y, 2-z; (viii) 0.5-x, 0.5-y, 2-z; (ix) x, 1+y, z; (x) 0.5-x, 0.5+y, 1.5-z.					
SrSn(PO ₄) ₂					
Sr1—O3 ⁱ	2.599(3)	Sr1—O3	2.789(2)	Sn1—O4 ⁱ	1.983(2)
Sr1—O3 ⁱⁱ	2.599(3)	Sr1—O3 ⁱⁱⁱ	2.789(2)	Sn1—O4 ^{vi}	1.983(2)
Sr1—O2	2.640(2)	P1—O3	1.502(2)	Sn1—O1 ^{vii}	2.045(2)
Sr1—O2 ⁱⁱⁱ	2.640(2)	P1—O4	1.519(2)	Sn1—O1	2.045(2)

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Sr1—O1 ⁱⁱⁱ	2.654(2)	P1—O1	1.557(2)	Sn1—O2 ^{vii}	2.047(2)
Sr1—O1	2.654(2)	P1—O2 ^{viii}	1.558(2)	Sn1—O2	2.047(2)
O4 ⁱ —Sn1—O4 ^{vi}	180.00(13)	O4 ^{vi} —Sn1—O2 ^{vii}	88.61(8)	O2 ^{vii} —Sn1—O2	180.00(11)
O4 ⁱ —Sn1—O1 ^{vii}	92.07(7)	O1 ^{vii} —Sn1—O2 ^{vii}	83.79(9)	O3—P1—O4	117.10(12)
O4 ^{vi} —Sn1—O1 ^{vii}	87.93(7)	O1—Sn1—O2 ^{vii}	96.21(9)	O3—P1—O1	108.02(10)
O4 ⁱ —Sn1—O1	87.93(7)	O4 ⁱ —Sn1—O2	88.61(8)	O4—P1—O1	107.34(10)
O4 ^{vi} —Sn1—O1	92.07(7)	O4 ^{vi} —Sn1—O2	91.39(8)	O3—P1—O2 ^{viii}	109.25(10)
O1 ^{vii} —Sn1—O1	180.00(8)	O1 ^{vii} —Sn1—O2	96.21(9)	O4—P1—O2 ^{viii}	106.55(9)
O4 ⁱ —Sn1—O2 ^{vii}	91.39(8)	O1—Sn1—O2	83.79(9)	O1—P1—O2 ^{viii}	108.29(11)
(i) x, 1-y, -0.5+z; (ii) 1-x, 1-y, 1-z; (iii) 1-x, y, 0.5-z; (iv) x, -1+y, z; (v) 1-x, -1+y, 0.5-z; (vi) 0.5-x, -0.5+y, 0.5-z; (vii) 0.5-x, 0.5-y, -z; (viii) x, 1+y, z; (ix) 0.5-x, 0.5+y, 0.5-z.					
BaSn(PO ₄) ₂					
Ba1—O3 ⁱ	2.796(4)	Ba1—O3 ^{vii}	3.140(2)	Sn1—O1 ^x	2.038(3)
Ba1—O3 ⁱⁱ	2.796(4)	Ba1—O3	3.140(2)	Sn1—O1 ^{iv}	2.038(3)
Ba1—O1 ⁱⁱⁱ	2.803(3)	Ba1—O3 ^v	3.140(2)	P1—O3	1.504(4)
Ba1—O1 ^{iv}	2.803(3)	Sn1—O2 ⁱ	1.988(4)	P1—O2	1.525(4)
Ba1—O1	2.803(3)	Sn1—O2 ^{viii}	1.988(4)	P1—O1 ^{xii}	1.556(3)
Ba1—O1 ^v	2.803(3)	Sn1—O1	2.038(3)	P1—O1	1.556(3)
Ba1—O3 ^{vi}	3.140(2)	Sn1—O1 ^{ix}	2.038(3)		
O2 ⁱ —Sn1—O2 ^{viii}	180.000	O2 ^{viii} —Sn1—O1 ^x	88.17(11)	O1 ^x —Sn1—O1 ^{iv}	180.000
O2 ⁱ —Sn1—O1	88.17(11)	O1—Sn1—O1 ^x	95.96(15)	O3—P1—O2	117.1(2)
O2 ^{viii} —Sn1—O1	91.83(11)	O1 ^{ix} —Sn1—O1 ^x	84.04(15)	O3—P1—O1 ^{xii}	108.28(15)
O2 ⁱ —Sn1—O1 ^{ix}	91.83(11)	O2 ⁱ —Sn1—O1 ^{iv}	88.17(11)	O2—P1—O1 ^{xii}	107.44(14)

$O2^{viii}-Sn1-O1^{ix}$	88.17(11)	$O2^{viii}-Sn1-O1^{iv}$	91.83(11)	$O3-P1-O1$	108.28(15)
$O1-Sn1-O1^{ix}$	180.000(1)	$O1-Sn1-O1^{iv}$	84.04(15)	$O2-P1-O1$	107.44(14)
$O2^i-Sn1-O1^x$	91.83(11)	$O1^{ix}-Sn1-O1^{iv}$	95.96(15)	$O1^{xii}-P1-O1$	108.0(2)

(i) $-0.5+x, 0.5+y, z$; (ii) $0.5-x, 1.5-y, -z$; (iii) $-x, y, -z$; (iv) $x, 2-y, z$; (v) $-x, 2-y, -z$; (vi) $x, 1+y, z$; (vii) $-x, 1-y, -z$; (viii) $0.5-x, 1.5-y, 1-z$; (ix) $-x, 2-y, 1-z$; (x) $-x, y, 1-z$; (xi) $x, y, 1+z$; (xii) $x, 1-y, z$; (xiii) $x, -1+y, z$; (xiv) $0.5+x, -0.5+y, z$.

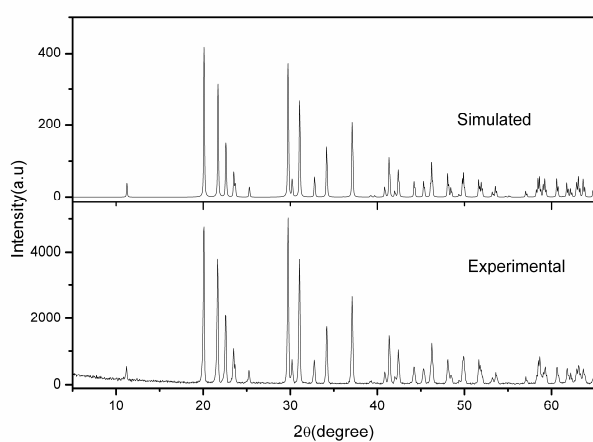


Figure S1. Experimental and simulated X-ray powder diffraction patterns of $BaSn(PO_4)_2$.

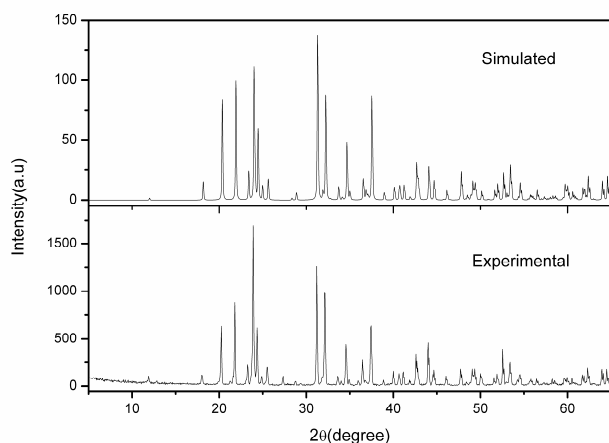


Figure S2. Experimental and simulated X-ray powder diffraction patterns of $SrTi(PO_4)_2$.

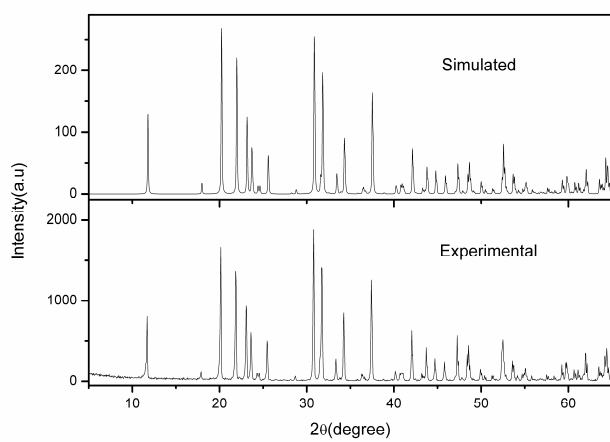


Figure S3. Experimental and simulated X-ray powder diffraction patterns of SrSn(PO₄)₂.