

Supporting Information for

Polymorphic Structures and Properties of Lead Chromium Phosphate $\text{Pb}_3\text{Cr}_2(\text{PO}_4)_4$

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Contents for Supporting Information:

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $\text{Pb}_3\text{Cr}_2(\text{PO}_4)_4$

	Atom	Symmetry	X	Y	Z	U_{eq}
Monoclinic $\text{Pb}_3\text{Cr}_2(\text{PO}_4)_4$	Pb(1)	4e	0.29942(10)	0.20696(9)	0.52656(9)	0.0120(4)
	Pb(2)	2a	0.0000	0.5000	0.5000	0.0090(4)
	Cr(3)	4e	0.2476(4)	0.6307(4)	0.2446(4)	0.0043(7)
	P(6)	4e	0.5745(6)	0.0897(6)	0.8581(6)	0.0053(10)
	P(7)	4e	-0.0197(6)	0.1379(6)	0.6554(6)	0.0040(10)
	O(1)	4e	0.1609(18)	0.5918(17)	0.0125(17)	0.008(3)
	O(2)	4e	0.0937(18)	0.7068(15)	0.7385(17)	0.006(3)

	O(3)	4e	0.5896(19)	0.2170(16)	0.7557(18)	0.008(3)
	O(11)	4e	0.3881(18)	0.0442(16)	0.7577(17)	0.007(3)
	O(13)	4e	0.0840(19)	0.4955(17)	0.2574(18)	0.010(3)
	O(21)	4e	0.3894(19)	0.6488(17)	0.4789(18)	0.010(3)
	O(22)	4e	0.1033(19)	0.2462(18)	0.6345(17)	0.009(3)
	O(23)	4e	0.3135(19)	0.4588(18)	0.6298(18)	0.013(3)
Tetragonal	Pb(1)	8b	0.07594(16)	0.34356(15)	0.26362(8)	0.0123(6)
Pb ₃ Cr ₂ (PO ₄) ₄	Pb(2)	4b	0.13418(16)	0.13418(16)	0.0000	0.0098(8)
	Cr(1)	8b	0.5006(6)	0.2643(5)	0.1213(4)	0.0050(12)
	P(1)	8b	0.2751(10)	-0.0056(9)	0.1714(5)	0.0066(17)
	P(2)	8b	-0.0446(10)	0.2261(9)	0.4292(5)	0.0047(17)
	O(3)	8b	0.628(3)	0.082(3)	0.1186(14)	0.007(5)
	O(4)	8b	0.330(3)	0.126(2)	0.1179(13)	0.005(5)
	O(5)	8b	0.666(3)	0.421(3)	0.1277(13)	0.008(5)
	O(6)	8b	0.515(2)	0.229(2)	0.2382(13)	0.010(5)
	O(7)	8b	0.324(3)	0.380(3)	0.3152(14)	0.011(5)
	O(8)	8b	0.110(3)	0.594(3)	0.3126(14)	0.012(5)
	O(9)	8b	0.354(3)	0.427(3)	0.1286(14)	0.009(5)
	O(10)	8b	0.544(3)	0.290(3)	0.0022(14)	0.015(5)

Table S2. Selected bond distances (Å) and angles (°) in tetragonal and monoclinic Pb₃Cr₂(PO₄)₄

	Distance	d (Å)	Distance	d (Å)
Tetragonal	Pb(1)—O(8)	2.40(3)	Cr(1)—O(6)	1.96(2)
Pb ₃ Cr ₂ (PO ₄) ₄	Pb(1)—O(7)	2.40(2)	Cr(1)—O(4)	1.96(2)

Pb(1)–O(3)	2.42(2)	Cr(1)–O(10)	2.02(3)
Pb(1)–O(5)	2.46(2)	Cr(1)–O(9)	1.96(2)
Pb(1)–P(2)	3.121(8)	Cr(1)–O(3)	1.99(2)
Pb(1)–Pb(2)	3.6788(13)	Cr(1)–O(5)	2.04(2)
Pb(2)–O(8) ×2	2.54(2)	P(1)–O(10)	1.52(3)
Pb(2)–O(7) ×2	2.55(2)	P(1)–O(9)	1.54(2)
Pb(2)–O(4) ×2	2.62(2)	P(1)–O(8)	1.52(2)
Pb(2)–O(9) ×2	2.73(2)	P(1)–O(4)	1.55(2)
Pb(2)–Pb(1) ×2	3.6788(13)	P(2)–O(7)	1.51(2)
		P(2)–O(3)	1.56(2)
		P(2)–O(5)	1.49(2)
		P(2)–O(6)	1.51(2)
O(8)–Pb(1)–O(7)	68.8(8)	O(8)–Pb(2)–O(8)	115.0(11)
O(8)–Pb(1)–O(3)	72.8(8)	O(8)–Pb(2)–O(7) ×2	179.0(7)
O(8)–Pb(1)–O(5)	110.0(8)	O(8)–Pb(2)–O(7) ×2	64.4(8)
O(7)–Pb(1)–O(3)	103.9(8)	O(8)–Pb(2)–O(4) ×2	79.5(7)
O(7)–Pb(1)–O(5)	78.8(8)	O(8)–Pb(2)–O(4) ×2	72.3(7)
O(3)–Pb(1)–O(5)	57.1(7)	O(8)–Pb(2)–O(9) ×2	99.5(7)
O(8)–Pb(1)–P(2)	93.5(6)	O(8)–Pb(2)–O(9) ×2	108.6(7)
O(7)–Pb(1)–P(2)	93.1(6)	O(7)–Pb(2)–O(7) ×2	116.2(11)
O(3)–Pb(1)–P(2)	29.3(5)	O(7)–Pb(2)–O(4) ×2	101.1(7)
O(5)–Pb(1)–P(2)	28.0(6)	O(7)–Pb(2)–O(4) ×2	106.7(7)
O(8)–Pb(1)–Pb(2)	43.4(6)	O(7)–Pb(2)–O(9) ×2	79.9(7)
O(7)–Pb(1)–Pb(2)	43.5(6)	O(7)–Pb(2)–O(9) ×2	72.4(7)
O(3)–Pb(1)–Pb(2)	112.8(6)	O(4)–Pb(2)–O(4)	126.1(10)

O(5)–Pb(1)–Pb(2)	119.7(5)	O(4)–Pb(2)–O(9) ×2	178.9(7)
P(2)–Pb(1)–Pb(2)	122.34(16)	O(4)–Pb(2)–O(9) ×2	53.8(7)
O(6)–Cr(1)–O(9)	95.7(10)	O(8)–Pb(2)–Pb(1) ×2	40.4(6)
O(6)–Cr(1)–O(3)	81.7(10)	O(8)–Pb(2)–Pb(1) ×2	139.7(6)
O(6)–Cr(1)–O(5)	90.7(9)	O(7)–Pb(2)–Pb(1) ×2	139.5(6)
O(6)–Cr(1)–O(4)	88.7(9)	O(7)–Pb(2)–Pb(1) ×2	40.4(6)
O(6)–Cr(1)–O(10)	165.1(10)	O(4)–Pb(2)–Pb(1) ×2	116.5(5)
O(9)–Cr(1)–O(4)	86.9(10)	O(4)–Pb(2)–Pb(1) ×2	63.6(5)
O(9)–Cr(1)–O(3)	172.6(11)	O(9)–Pb(2)–Pb(1) ×2	62.4(5)
O(9)–Cr(1)–O(5)	88.5(10)	O(9)–Pb(2)–Pb(1) ×2	117.5(5)
O(9)–Cr(1)–O(10)	96.0(10)	Pb(1)–Pb(2)–Pb(1)	179.85(9)
O(4)–Cr(1)–O(10)	101.0(10)		
O(4)–Cr(1)–O(5)	175.3(10)		
O(4)–Cr(1)–O(3)	86.0(10)		
O(3)–Cr(1)–O(5)	98.5(11)		
O(3)–Cr(1)–O(10)	87.7(10)		
O(10)–Cr(1)–O(5)	80.4(10)		
O(8)–P(1)–O(9)	115.5(14)	O(7)–P(2)–O(6)	112.3(14)
O(8)–P(1)–O(4)	108.6(14)	O(7)–P(2)–O(3)	112.8(14)
O(10)–P(1)–O(8)	108.6(14)	O(6)–P(2)–O(3)	108.1(13)
O(10)–P(1)–O(4)	113.5(13)	O(5)–P(2)–O(6)	110.4(13)
O(10)–P(1)–O(9)	107.4(13)	O(5)–P(2)–O(3)	99.7(13)
O(9)–P(1)–O(4)	103.3(12)	O(5)–P(2)–O(7)	112.6(14)
P(1)–O(4)–Cr(1)	134.9(14)	P(2)–O(5)–Cr(1)	142.9(15)
P(1)–O(9)–Cr(1)	139.4(15)	P(2)–O(3)–Cr(1)	131.7(14)

	P(1)—O(10)—Cr(1)	139.2(16)	P(2)—O(6)—Cr(1)	145.4(15)
Monoclinic Pb ₃ Cr ₂ (PO ₄) ₄	Pb(1)—O(22)	2.401(15)	Cr(3)—O(13)	1.943(16)
	Pb(1)—O(23)	2.433(16)	Cr(3)—O(21)	1.964(15)
	Pb(1)—O(11)	2.409(14)	Cr(3)—O(2)	1.986(15)
	Pb(1)—O(3)	2.505(15)	Cr(3)—O(1)	1.959(15)
	Pb(2)—O(23) ×2	2.529(16)	Cr(3)—O(11)	1.978(15)
	Pb(2)—O(13) ×2	2.667(15)	Cr(3)—O(3)	1.996(15)
	Pb(2)—O(22) ×2	2.559(16)		
	Pb(2)—O(2) ×2	2.710(14)		
	P(7)—O(2)	1.539(15)	P(6)—O(21)	1.490(15)
	P(7)—O(13)	1.547(16)	P(6)—O(3)	1.527(15)
	P(7)—O(22)	1.542(16)	P(6)—O(23)	1.513(17)
	P(7)—O(1)	1.552(15)	P(6)—O(11)	1.553(15)
	O(22)—Pb(1)—O(11)	74.3(5)	O(11)—Pb(1)—O(23)	106.0(5)
	O(22)—Pb(1)—O(23)	67.6(5)	O(11)—Pb(1)—O(3)	57.9(5)
	O(22)—Pb(1)—O(3)	108.3(5)	O(23)—Pb(1)—O(3)	77.5(5)
	O(22)—Pb(1)—P(6)	92.3(4)	O(22)—Pb(1)—Pb(2)	43.8(4)
	O(11)—Pb(1)—P(6)	29.1(4)	O(11)—Pb(1)—Pb(2)	115.5(3)
	O(23)—Pb(1)—P(6)	92.8(4)	O(23)—Pb(1)—Pb(2)	43.2(4)
	O(3)—Pb(1)—P(6)	28.9(3)	O(3)—Pb(1)—Pb(2)	118.4(3)
P(6)—Pb(1)—Pb(2)	122.22(10)			
O(23)—Pb(2)—O(22) ×2	63.8(5)	O(23)—Pb(2)—Pb(1) ×2	41.2(4)	
O(23)—Pb(2)—O(22) ×2	116.2(5)	O(23)—Pb(2)—Pb(1) ×2	138.8(4)	
O(23)—Pb(2)—O(13) ×2	74.1(5)	O(22)—Pb(2)—Pb(1) ×2	40.5(3)	
O(23)—Pb(2)—O(13) ×2	105.9(5)	O(22)—Pb(2)—Pb(1) ×2	139.5(3)	

O(22)–Pb(2)–O(13) ×2	102.6(5)	O(13)–Pb(2)–Pb(1) ×2	64.8(3)
O(22)–Pb(2)–O(13) ×2	77.4(5)	O(13)–Pb(2)–Pb(1) ×2	115.2(3)
O(23)–Pb(2)–O(2) ×2	99.0(5)	O(2)–Pb(2)–Pb(1) ×2	61.0(3)
O(23)–Pb(2)–O(2) ×2	81.0(5)	O(2)–Pb(2)–Pb(1) ×2	119.0(3)
O(22)–Pb(2)–O(2) ×2	72.5(4)	O(23)–Pb(2)–O(23)	180.000(2)
O(22)–Pb(2)–O(2) ×2	107.5(4)	O(22)–Pb(2)–O(22)	180.000(2)
O(13)–Pb(2)–O(2) ×2	53.5(4)	O(13)–Pb(2)–O(13)	180.000(1)
O(13)–Pb(2)–O(2) ×2	126.5(4)	O(2)–Pb(2)–O(2)	180.000(1)
O(13)–Cr(3)–O(1)	91.1(6)	O(21)–Cr(3)–O(11)	85.5(6)
O(13)–Cr(3)–O(21)	96.5(6)	O(21)–Cr(3)–O(2)	93.7(6)
O(13)–Cr(3)–O(11)	88.6(6)	O(13)–Cr(3)–O(2)	86.0(6)
O(1)–Cr(3)–O(21)	164.8(7)	O(13)–Cr(3)–O(3)	174.6(6)
O(1)–Cr(3)–O(11)	81.5(6)	O(11)–Cr(3)–O(2)	174.4(6)
O(1)–Cr(3)–O(2)	99.9(6)	O(11)–Cr(3)–O(3)	95.7(6)
O(1)–Cr(3)–O(3)	92.8(6)	O(2)–Cr(3)–O(3)	89.6(6)
O(21)–Cr(3)–O(3)	80.6(6)		
O(21)–P(6)–O(3)	108.8(9)	O(3)–P(6)–O(11)	101.3(8)
O(21)–P(6)–O(11)	112.6(8)	O(23)–P(6)–O(3)	112.7(9)
O(21)–P(6)–O(23)	111.5(9)	O(23)–P(6)–O(11)	109.6(9)
O(2)–P(7)–O(22)	111.2(8)	O(22)–P(7)–O(13)	107.3(9)
O(2)–P(7)–O(13)	103.5(8)	O(22)–P(7)–O(1)	110.3(8)
O(2)–P(7)–O(1)	110.8(8)	O(13)–P(7)–O(1)	113.5(8)
P(7)–O(1)–Cr(3)	142.3(9)	P(6)–O(11)–Cr(3)	136.5(9)
P(7)–O(2)–Cr(3)	140.1(9)	P(6)–O(21)–Cr(3)	145.6(10)
P(7)–O(13)–Cr(3)	134.9(9)	P(6)–O(3)–Cr(3)	141.2(10)