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Tailoring the Photoluminescence Properties of Transition Metal Phosphonates

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for silver *m*-phosphonobenzoate, $Ag_6(O_3PC_6H_4CO_2)_2$.

	x	y	z	U(eq)
Ag(1)	4976(1)	1232(1)	3671(1)	17(1)
Ag(2)	3075(1)	2889(1)	4318(1)	22(1)
Ag(3)	5048(1)	1306(1)	2709(1)	26(1)
Ag(4)	9709(1)	1114(1)	4859(1)	19(1)
Ag(5)	4490(1)	1428(1)	4949(1)	19(1)
Ag(6)	7115(1)	-213(1)	4410(1)	22(1)
O(1)	8383(5)	1424(3)	-527(2)	19(1)
O(2)	3372(5)	2697(3)	5313(1)	17(1)
O(3)	5462(5)	2180(2)	4322(1)	13(1)
O(4)	2912(5)	2076(3)	3577(2)	22(1)
O(5)	2368(5)	1840(3)	2844(1)	17(1)
O(6)	4528(4)	385(2)	4411(1)	11(1)
O(7)	6337(5)	1116(2)	5533(1)	14(1)
O(8)	1686(5)	18(3)	4748(1)	16(1)
O(9)	7162(5)	450(3)	3627(1)	18(1)
O(10)	7642(5)	710(3)	2896(2)	21(1)
P(1)	2069(2)	2306(1)	5623(1)	11(1)
P(2)	3038(2)	-224(1)	4409(1)	10(1)
C(1)	2988(7)	2230(4)	6180(2)	11(1)
C(2)	4545(8)	2574(4)	6270(2)	14(1)
C(3)	252(7)	2467(4)	3300(2)	12(1)
C(4)	4336(8)	2160(4)	7045(2)	15(2)
C(5)	2771(8)	1826(4)	6960(2)	22(2)
C(6)	2093(8)	1863(4)	6531(2)	17(2)
C(7)	1978(8)	2105(4)	3229(2)	13(1)
C(8)	2140(7)	-200(4)	3850(2)	11(1)
C(9)	537(7)	117(4)	3769(2)	11(1)
C(10)	9849(7)	128(4)	3339(2)	15(1)
C(11)	10801(8)	-179(4)	2986(2)	17(2)
C(12)	2414(7)	-483(4)	3052(2)	21(2)
C(13)	3067(8)	-506(4)	3488(2)	18(2)
C(14)	8086(8)	461(4)	3274(2)	14(1)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.