Attachments as ESI of the manuscript entitled "Crystallographic, optical and dielectric properties of gel grown Praseodymium malonate single crystals".

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Table 3 (a).

Crystallographic data of Pr $(C_3H_2O_4)_3$ $(H_2O)_6$.

Empirical formula	C9 H18 O18 Pr2
Formula weight	685.97
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2/m
Unit cell dimensions	a = 15.107(9) Å
	b = 11.976(5) Å
	c = 10.343(7) Å
	β = 121.508
Volume	1871.2704(2) $Å^3$
Z	4
Calculated density	2.379 Mg/m^3
Absorption coefficient	5.115 mm^{-1}
F_{000}	1296
Crystal size	0.35 x 0.30 x 0.25 mm
Theta range for data collection	2.97 to 28.21 deg.

Index ranges	-21<=h<=22
	-16<=k<=16
	-14<=l<=9
Reflections collected / unique	7511 / 2349 [R(int) = 0.0416]
Completeness to theta =	28.21 99.4 %
Max. and min. transmission	0.3612 and 0.2676
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2349/6 /149
Goodness-of-fit on F^2	1.116
Final R indices [I>2σ(I)]	R1 = 0.0224, wR2 = 0.0588
R indices (all data)	R1 = 0.0235, wR2 = 0.0597
Extinction coefficient	0.00297(13)
Largest diff. peak and hole	1.048 and -0.882 e.A^{-3}

Table 3 (b).

Atomic coordination and equivalent thermal parameters.

Atoms	x	y	z	Ueq
C(1)	1386(2)	2109(2)	3323(3)	19(1)
C(2)	1184(3)	3278(3)	2801(4)	25(1)
C(3)	4256(2)	2001(2)	1250(3)	17(1)
C(4)	5000	1251(4)	2500	20(1)
C(5)	3127(2)	-1178(2)	2419(3)	19(1)
O(1)	1625(2)	1445(2)	2741(3)	26(1)
O(2)	1278(2)	1847(2)	4277(3)	34(1)
O(3)	3417(2)	2092(2)	916(2)	20(1)
O(4)	4507(2)	2563(2)	608(3)	27(1)
O(5)	3756(2)	1792(2)	3844(3)	29(1)
O(6)	1821(3)	628(2)	-1134(4)	41(1)
O(7)	830(2)	26(2)	34(5)	55(1)
O(8)	3003(2)	-189(2)	2149(3)	34(1)
O(9)	2751(2)	-1690(2)	2905(3)	23(1)
Pr(1)	2166(1)	1469(1)	1199(1)	14(1)

Table 3 (c)

Bond lengths (Å)

Atom	length
C(1)-O(2)	1.239(4)
C(1)-O(1)	1.267(4)
C(1)-C(2)	1.525(4)
C(2)-C(5)#1	1.515(4)
C(3)-O(4)	1.257(4)
C(3)-O(3)	1.262(3)
C(3)-C(4)	1.516(4)
C(3)-Pr(1)#2	2.999(3)
C(4)-C(3)#3	1.516(4)
C(5)-O(9)	1.249(4)
C(5)-O(8)	1.252(4)
C(5)-C(2)#4	1.515(4)
O(1)-Pr(1)	2.420(2)
O(3)-Pr(1)	2.493(2)
O(3)-Pr(1)#2	2.636(2)
O(4)-Pr(1)#2	2.604(2)

O(5)-Pr(1)	2.570(3)
O(6)-Pr(1)	2.534(3)
O(7)-Pr(1)	2.566(3)
O(8)-Pr(1)	2.366(2)
O(9)-Pr(1)#4	2.468(2)
Pr(1)-O(9)#1	2.468(2)
Pr(1)-O(4)#2	2.604(2)
Pr(1)-O(3)#2	2.636(2)
Pr(1)-C(3)#2	2.999(3)

Table 3 (d).

Bond angles (degree)

Atoms	Angle
O(2)-C(1)-O(1)	123.0(3)
O(2)-C(1)-C(2)	117.5(3)
O(1)-C(1)-C(2)	119.5(3)
C(5)#1-C(2)-C(1)	117.9(3)
O(4)-C(3)-O(3)	121.1(3)
O(4)-C(3)-C(4)	118.6(2)
O(3)-C(3)-C(4)	120.2(2)
O(4)-C(3)-Pr(1)#2	59.81(16)
O(3)-C(3)-Pr(1)#2	61.29(15)
C(4)-C(3)-Pr(1)#2	178.2(2)
C(3)-C(4)-C(3)#3	104.1(3)
O(9)-C(5)-O(8)	123.2(3)
O(9)-C(5)-C(2)#4	121.1(3)
O(8)-C(5)-C(2)#4	115.7(3)
C(1)-O(1)-Pr(1)	138.67(19)
C(3)-O(3)-Pr(1)	149.7(2)
C(3)-O(3)-Pr(1)#2	93.89(17)

Pr(1)-O(3)-Pr(1)#2	116.15(8)
C(3)-O(4)-Pr(1)#2	95.53(18)
C(5)-O(8)-Pr(1)	158.6(2)
C(5)-O(9)-Pr(1)#4	137.2(2)
O(8)-Pr(1)-O(1)	93.61(8)
O(8)-Pr(1)-O(9)#1	139.04(9)
O(1)-Pr(1)-O(9)#1	70.79(7)
O(8)-Pr(1)-O(3)	89.30(8)
O(1)-Pr(1)-O(3)	147.04(8)
O(9)#1-Pr(1)-O(3)	85.69(7)
O(8)-Pr(1)-O(6)	78.58(10)
O(1)-Pr(1)-O(6)	141.85(9)
O(9)#1-Pr(1)-O(6)	136.30(9)
O(3)-Pr(1)-O(6)	70.82(8)
O(8)-Pr(1)-O(7)	74.63(10)
O(1)-Pr(1)-O(7)	74.74(10)
O(9)#1-Pr(1)-O(7)	131.84(8)
O(3)-Pr(1)-O(7)	137.13(9)
O(6)-Pr(1)-O(7)	67.16(10)
O(8)-Pr(1)-O(5)	71.60(9)
O(1)-Pr(1)-O(5)	77.31(9)
O(9)#1-Pr(1)-O(5)	68.12(8)
O(3)-Pr(1)-O(5)	72.52(8)

O(6)-Pr(1)-O(5)	132.38(9)
O(7)-Pr(1)-O(5)	134.10(12)
O(8)-Pr(1)-O(4)#2	146.89(9)
O(1)-Pr(1)-O(4)#2	80.47(8)
O(9)#1-Pr(1)-O(4)#2	69.62(8)
O(3)-Pr(1)-O(4)#2	113.27(7)
O(6)-Pr(1)-O(4)#2	86.16(10)
O(7)-Pr(1)-O(4)#2	72.38(10)
O(5)-Pr(1)-O(4)#2	136.71(8)
O(8)-Pr(1)-O(3)#2	142.24(8)
O(1)-Pr(1)-O(3)#2	123.53(7)
O(9)#1-Pr(1)-O(3)#2	68.57(7)
O(3)-Pr(1)-O(3)#2	63.85(8)
O(6)-Pr(1)-O(3)#2	68.05(8)
O(7)-Pr(1)-O(3)#2	106.42(11)
O(5)-Pr(1)-O(3)#2	119.34(8)
O(4)#2-Pr(1)-O(3)#2	49.48(6)
O(8)-Pr(1)-C(3)#2	154.22(9)
O(1)-Pr(1)-C(3)#2	101.97(8)
O(9)#1-Pr(1)-C(3)#2	66.35(8)
O(3)-Pr(1)-C(3)#2	88.62(7)
O(6)-Pr(1)-C(3)#2	76.48(9)
O(7)-Pr(1)-C(3)#2	89.69(11)

O(5)-Pr(1)-C(3)#2	131.65(8)
O(4)#2-Pr(1)-C(3)#2	24.66(7)
O(3)#2-Pr(1)-C(3)#2	24.83(7)

Symmetry transformations used to generate equivalent atoms:

(1 -x+1/2, y+1/2,-z+1/2) #2 (-x+1/2, -y+1/2,-z)

#3 (-x+1, y,-z+1/2) and #4 (-x+1/2,y-1/2,-z+1/2)

Table 3(e).

Anisotropic displacement parameters ($A^2 \times 10^3$) for PMH

The anisotropic displacement factor exponent takes the form:

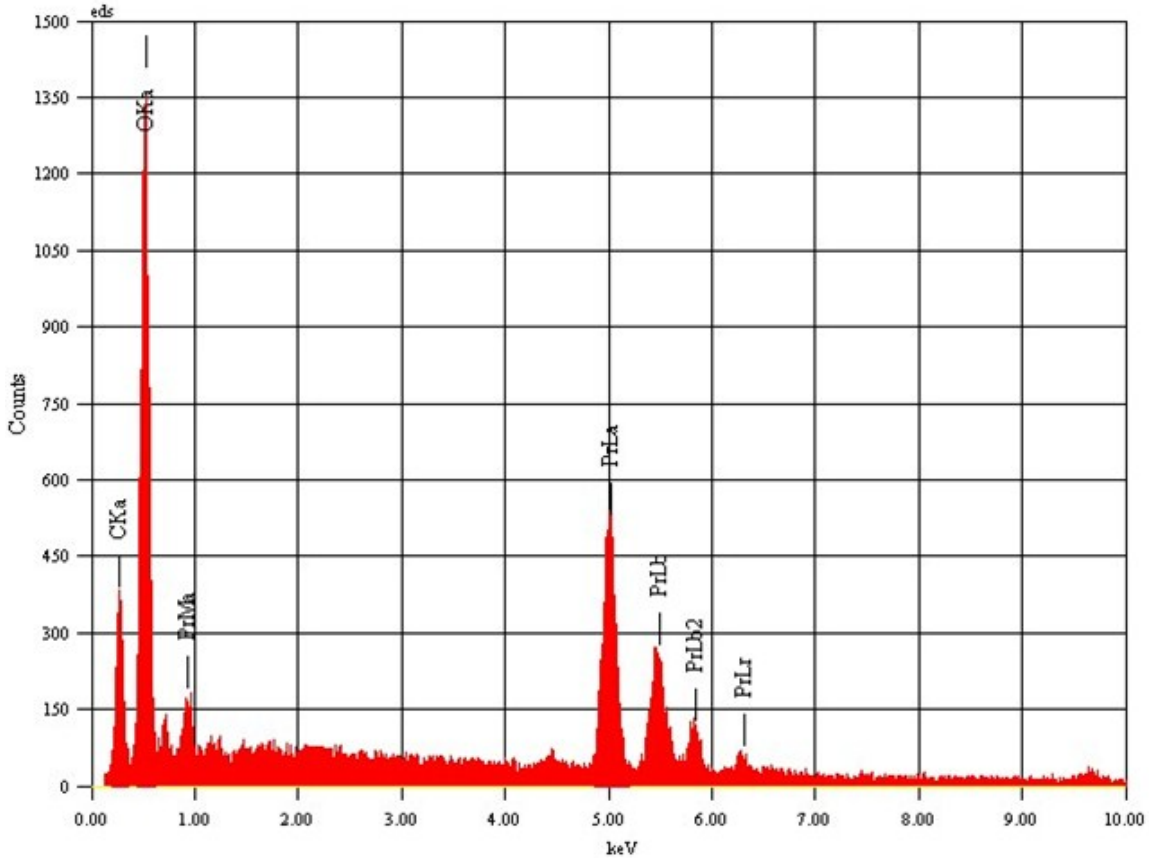
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

Atoms	U11	U22	U33	U23	U13	U12
C(1)	24(1)	17(1)	23(1)	0(1)	18(1)	0(1)
C(2)	39(2)	16(1)	37(2)	4(1)	32(2)	5(1)
C(3)	17(1)	18(1)	16(1)	-3(1)	10(1)	-2(1)
C(4)	15(2)	19(2)	19(2)	0	8(2)	0
C(5)	25(1)	14(1)	17(1)	0(1)	12(1)	1(1)
O(1)	47(2)	14(1)	37(2)	1(1)	36(1)	2(1)
O(2)	62(2)	24(1)	40(2)	2(1)	44(2)	2(1)
O(3)	17(1)	27(1)	20(1)	3(1)	13(1)	2(1)
O(4)	21(1)	36(1)	27(1)	9(1)	16(1)	2(1)
O(5)	26(1)	39(1)	24(1)	-8(1)	17(1)	0(1)
O(6)	79(2)	22(1)	56(2)	-17(1)	58(2)	-18(1)
O(7)	56(2)	35(2)	107(3)	-35(2)	66(2)	-23(1)
O(8)	47(2)	14(1)	50(2)	7(1)	34(1)	6(1)
O(9)	33(1)	17(1)	28(1)	3(1)	24(1)	4(1)
Pr(1)	20(1)	11(1)	19(1)	0(1)	15(1)	0(1)

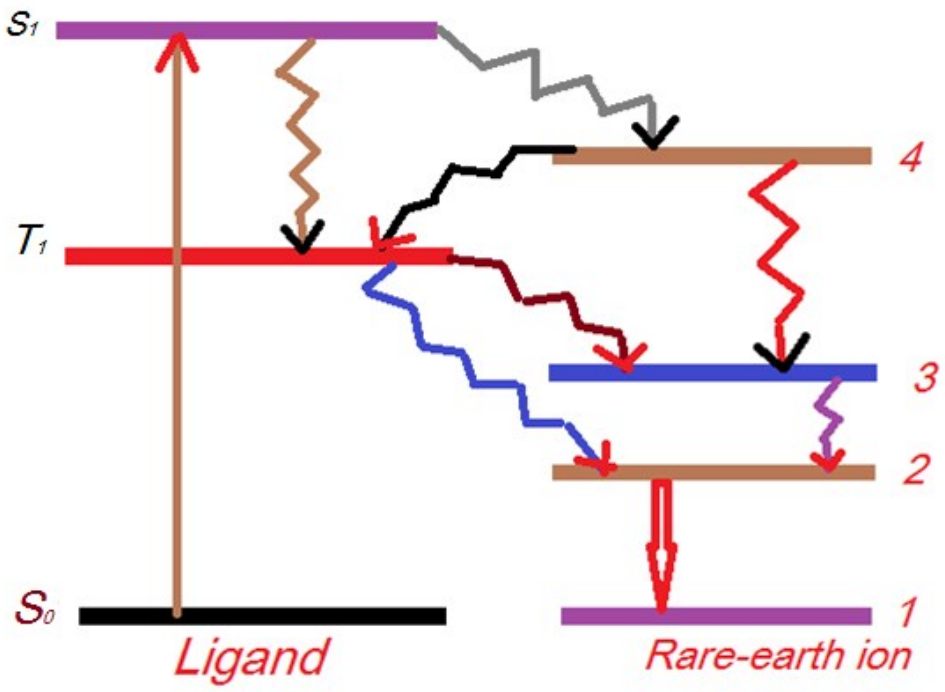
Table 3 (f).

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for PMH.

Atoms	x	y	z	U(eq)
H(5A)	4180(30)	2040(40)	3790(70)	80(20)
H(5B)	3680(40)	2200(40)	4360(60)	75(19)
H(6A)	2090(40)	900(40)	-1500(60)	69(18)
H(6B)	1750(40)	-36(17)	-1340(50)	51(14)



EDAX pattern showing peaks corresponding to Pr, carbon and oxygen.



Schematic diagram depicting antenna effect in Pr^{3+} co-ordinated with organic ligand (malonic acid).