Supporting Information

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A novel samarium(III) orotate complex $[NaSm(orotate)_4(H_2O)_{10}]\cdot 3H_2O$ - crystal structure and vibrational spectra

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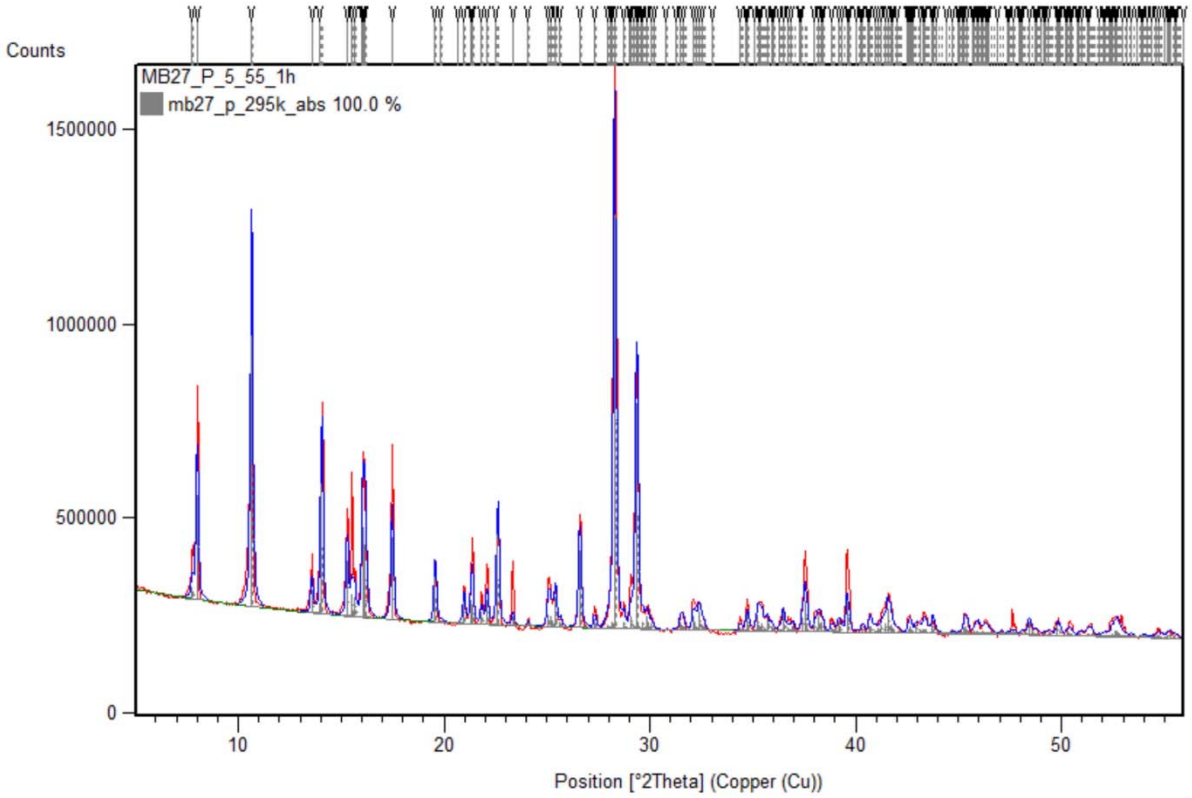

Figure S1: Experimental PXRD pattern for $[NaSm(orotate)_4(H_2O)_{10}]\cdot 3H_2O$ (red line) and Rietveld-fitted theoretical pattern (blue line) generated from single crystal data.

Table S1: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sm1	0	0.85267(2)	0.42830(3)	0.02029(7)	
Na1	0.10691(18)	0.2935(3)	0.5555(4)	0.0497(11)	0.5
O1W	0	1.0291(3)	0.3476(4)	0.0393(11)	
H1W	0.0296(18)	1.062(4)	0.322(4)	0.059*	
O2W	0	0.7887(3)	0.6193(3)	0.0310(10)	
H2W	0.0295(16)	0.815(4)	0.648(4)	0.047*	
O3W	0.06456(14)	0.9712(3)	0.5246(3)	0.0414(8)	
H3WA	0.0982(15)	0.950(4)	0.519(5)	0.062*	
H3WB	0.067(2)	1.034(2)	0.528(4)	0.062*	
O4W	0	0.6856(4)	0.3313(4)	0.0438(13)	
H4W	0.0316(17)	0.663(4)	0.310(4)	0.066*	
O5W	0.07261(14)	0.8678(2)	0.2820(3)	0.0357(8)	
H5WA	0.094(2)	0.817(3)	0.275(4)	0.054*	
H5WB	0.090(2)	0.925(3)	0.273(4)	0.054*	
O6W	0	0.5602(5)	0.6094(5)	0.0677(16)	
H6WA	0	0.6290(17)	0.603(9)	0.102*	
H6WB	0.015(6)	0.524(6)	0.554(7)	0.102*	0.5
O7W	0.0242(3)	0.1819(5)	0.5809(6)	0.0504(18)	0.5
O8W	0.0818(3)	0.4201(6)	0.6990(7)	0.0413(18)	0.5
H8WA	0.065(4)	0.478(6)	0.685(13)	0.062*	0.5
H8WB	0.112(3)	0.449(9)	0.727(8)	0.062*	0.5
O10W	0.0369(4)	0.4091(8)	0.4452(11)	0.097(3)	0.5
O13	0.16219(13)	0.8519(2)	0.5037(3)	0.0404(8)	
O11W	−0.0681(4)	0.2863(9)	0.4622(12)	0.120(6)	0.5
O12	0.33276(13)	0.6372(2)	0.5050(3)	0.0404(8)	
O11	0.08630(11)	0.7455(2)	0.4748(2)	0.0276(6)	

O14	0.19009(14)	0.3908(2)	0.4995(3)	0.0382(8)	
O23	0.34334(13)	0.4710(2)	0.7529(3)	0.0390(8)	
O22	0.16551(12)	0.2678(2)	0.7456(3)	0.0344(7)	
O21	0.41455(13)	0.3522(2)	0.7649(3)	0.0352(7)	
O24	0.30338(13)	0.0113(2)	0.7517(3)	0.0321(7)	
N11	0.23818(14)	0.6932(3)	0.4990(3)	0.0246(7)	
H11	0.248672	0.758306	0.500630	0.029*	
N13	0.25957(15)	0.5160(3)	0.5010(3)	0.0280(8)	
H13	0.285099	0.466315	0.502720	0.034*	
N21	0.26075(14)	0.3168(3)	0.7461(3)	0.0227(7)	
H21	0.251456	0.382373	0.741938	0.027*	
N23	0.23569(15)	0.1406(2)	0.7513(3)	0.0245(7)	
H23	0.209142	0.092694	0.753291	0.029*	
C12	0.28057(18)	0.6172(3)	0.5018(3)	0.0260(9)	
C14	0.20220(18)	0.4857(3)	0.4979(3)	0.0262(9)	
C15	0.16105(17)	0.5695(3)	0.4934(3)	0.0245(9)	
H15	0.121313	0.554821	0.490236	0.029*	
C16	0.17988(17)	0.6704(3)	0.4936(3)	0.0212(8)	
C17	0.13921(17)	0.7640(3)	0.4904(3)	0.0240(9)	
C22	0.21699(16)	0.2435(3)	0.7473(3)	0.0229(8)	
C24	0.29268(18)	0.1068(3)	0.7526(3)	0.0242(9)	
C25	0.33530(18)	0.1886(3)	0.7544(3)	0.0255(9)	
H25	0.374764	0.171812	0.757750	0.031*	
C26	0.31835(17)	0.2908(3)	0.7514(3)	0.0215(8)	
C27	0.36229(18)	0.3796(3)	0.7563(3)	0.0245(9)	
O9W	−0.0744(4)	0.4682(8)	0.7617(8)	0.065(2)	0.5

Table S2: Atomic displacement parameters (Å^2).

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sm1	0.01425(11)	0.01598(11)	0.03065(12)	0	0	0.0003(2)
Na1	0.039(2)	0.034(2)	0.076(3)	0.0025(19)	0.007(2)	0.0000(19)
O1W	0.025(2)	0.030(3)	0.064(3)	0	0	0.020(2)
O2W	0.023(2)	0.035(3)	0.036(2)	0	0	−0.004(2)
O3W	0.0304(17)	0.0241(16)	0.070(2)	0.0000(15)	−0.0115(18)	−0.0063(17)
O4W	0.023(2)	0.036(3)	0.072(4)	0	0	−0.028(3)
O5W	0.0286(18)	0.0260(18)	0.053(2)	0.0032(14)	0.0128(15)	0.0067(15)
O6W	0.067(4)	0.047(3)	0.089(5)	0	0	0.016(3)
O7W	0.056(4)	0.044(4)	0.050(4)	−0.004(3)	0.001(3)	−0.008(3)
O8W	0.030(4)	0.036(4)	0.058(5)	0.002(3)	0.001(4)	0.006(4)
O10W	0.089(6)	0.120(8)	0.082(9)	−0.014(6)	0.007(7)	−0.001(8)
O13	0.0207(16)	0.0182(15)	0.082(2)	−0.0005(13)	−0.0077(16)	−0.0026(15)
O11W	0.048(5)	0.104(8)	0.209(19)	0.010(5)	−0.042(8)	−0.048(9)
O12	0.0193(16)	0.0374(19)	0.065(2)	0.0029(14)	−0.0021(15)	0.0064(16)
O11	0.0157(13)	0.0231(14)	0.0441(16)	0.0010(12)	−0.0022(11)	0.0025(12)
O14	0.0378(19)	0.0222(16)	0.055(2)	−0.0034(15)	0.0005(16)	0.0014(15)
O23	0.0272(16)	0.0182(15)	0.071(2)	−0.0021(13)	0.0016(16)	−0.0011(15)
O22	0.0191(15)	0.0255(16)	0.059(2)	−0.0015(13)	0.0004(14)	0.0030(15)
O21	0.0178(15)	0.0282(16)	0.060(2)	−0.0011(13)	0.0011(14)	−0.0098(14)
O24	0.0306(16)	0.0164(15)	0.0493(18)	0.0004(13)	0.0012(14)	−0.0015(13)
N11	0.0206(18)	0.0177(17)	0.0354(19)	0.0021(15)	−0.0018(15)	−0.0003(15)
N13	0.0224(18)	0.0196(17)	0.042(2)	0.0077(15)	0.0012(16)	0.0011(15)
N21	0.0198(17)	0.0125(15)	0.0359(18)	0.0000(14)	0.0008(15)	−0.0030(14)
N23	0.0223(18)	0.0152(16)	0.0359(19)	−0.0028(14)	0.0021(15)	−0.0003(15)
C12	0.020(2)	0.027(2)	0.031(2)	0.0024(18)	0.0003(17)	0.0022(18)
C14	0.029(2)	0.020(2)	0.029(2)	−0.0011(18)	0.0023(18)	0.0000(17)
C15	0.0193(19)	0.023(2)	0.031(2)	−0.0011(17)	0.0002(16)	0.0002(17)
C16	0.0179(19)	0.025(2)	0.0205(19)	0.0033(17)	0.0002(15)	−0.0008(16)

C17	0.021(2)	0.024(2)	0.028(2)	0.0014(17)	0.0001(16)	0.0035(17)
C22	0.023(2)	0.020(2)	0.026(2)	−0.0013(17)	0.0022(17)	0.0002(17)
C24	0.027(2)	0.019(2)	0.026(2)	−0.0006(18)	0.0033(17)	0.0012(17)
C25	0.018(2)	0.023(2)	0.036(2)	0.0022(18)	0.0004(17)	−0.0005(18)
C26	0.021(2)	0.021(2)	0.0229(19)	−0.0025(16)	0.0030(16)	−0.0004(16)
C27	0.020(2)	0.022(2)	0.032(2)	−0.0023(17)	0.0032(17)	−0.0028(17)
O9W	0.036(5)	0.074(7)	0.085(7)	0.016(5)	0.004(5)	0.027(6)

Table S3: Geometric parameters (Å, deg).

Sm1—O1W	2.460(4)	O8W—H8WB	0.86(3)
Sm1—O2W	2.542(4)	O10W—O10W^{i}	1.689(19)
Sm1—O3W	2.434(3)	O13—C17	1.244(5)
Sm1—O3W^{i}	2.434(3)	O12—C12	1.223(5)
Sm1—O4W	2.447(5)	O11—C17	1.250(5)
Sm1—O5W	2.491(3)	O14—C14	1.235(5)
Sm1—O5W^{i}	2.491(3)	O23—C27	1.239(5)
Sm1—O11	2.470(3)	O22—C22	1.220(4)
Sm1—O11^{i}	2.470(3)	O21—C27	1.251(5)
Na1—O7W	2.387(8)	O24—C24	1.237(5)
Na1—O8W	2.487(10)	N11—H11	0.8600
Na1—O10W	2.581(13)	N11—C12	1.369(5)
Na1—O12^{ii}	2.500(5)	N11—C16	1.368(5)
Na1—O14	2.378(5)	N13—H13	0.8600
Na1—O22	2.766(6)	N13—C12	1.372(5)
O1W—H1W	0.86(3)	N13—C14	1.370(5)
O1W—H1W^{i}	0.86(3)	N21—H21	0.8600
O2W—H2W	0.84(3)	N21—C22	1.368(5)
O2W—H2W^{i}	0.84(3)	N21—C26	1.362(5)
O3W—H3WA	0.82(3)	N23—H23	0.8600
O3W—H3WB	0.80(3)	N23—C22	1.375(5)

O4W—H4W^{i}	0.82(3)	N23—C24	1.374(5)
O4W—H4W	0.82(3)	C14—C15	1.422(6)
O5W—H5WA	0.81(3)	C15—H15	0.9300
O5W—H5WB	0.84(3)	C15—C16	1.352(6)
O6W—H6WA	0.88(2)	C16—C17	1.510(6)
O6W—H6WB	0.91(3)	C24—C25	1.425(6)
O6W—H6WB^{i}	0.91(3)	C25—H25	0.9300
O7W—O7W^{i}	1.108(14)	C25—C26	1.354(5)
O8W—H8WA	0.85(3)	C26—C27	1.512(6)

O1W—Sm1—O2W	133.08(15)	Sm1—O4W—H4W	117(4)
O1W—Sm1—O5W	67.89(11)	Sm1—O4W—H4W^{i}	117(4)
O1W—Sm1—O5W^{i}	67.89(11)	H4W—O4W—H4W^{i}	123(9)
O1W—Sm1—O11	126.82(6)	Sm1—O5W—H5WA	115(4)
O1W—Sm1—O11^{i}	126.82(6)	Sm1—O5W—H5WB	119(4)
O3W^{i}—Sm1—O1W	69.15(13)	H5WA—O5W—H5WB	113(6)
O3W—Sm1—O1W	69.15(13)	H6WA—O6W—H6WB^{i}	116(9)
O3W—Sm1—O2W	74.01(12)	H6WA—O6W—H6WB	116(9)
O3W^{i}—Sm1—O2W	74.01(12)	H6WB—O6W—H6WB^{i}	44(10)
O3W—Sm1—O3W^{i}	74.86(17)	O7W^{i}—O7W—Na1	142.55(19)
O3W^{i}—Sm1—O4W	141.67(9)	Na1—O8W—H8WA	121(10)
O3W—Sm1—O4W	141.67(9)	Na1—O8W—H8WB	113(7)
O3W^{i}—Sm1—O5W^{i}	85.18(13)	H8WA—O8W—H8WB	95(10)
O3W—Sm1—O5W	85.18(13)	O10W^{i}—O10W—Na1	128.4(2)
O3W—Sm1—O5W^{i}	136.70(11)	C12—O12—Na1^{iii}	135.5(3)
O3W^{i}—Sm1—O5W	136.70(11)	C17—O11—Sm1	135.2(3)
O3W—Sm1—O11^{i}	135.08(12)	C14—O14—Na1	133.7(3)
O3W—Sm1—O11	74.64(11)	C22—O22—Na1	121.0(3)
O3W^{i}—Sm1—O11	135.08(12)	C12—N11—H11	118.5
O3W^{i}—Sm1—O11^{i}	74.64(11)	C16—N11—H11	118.5

O4W—Sm1—O1W	125.57(19)	C16—N11—C12	123.0(3)
O4W—Sm1—O2W	101.34(17)	C12—N13—H13	116.6
O4W—Sm1—O5W^{i}	72.35(12)	C14—N13—H13	116.6
O4W—Sm1—O5W	72.35(12)	C14—N13—C12	126.8(3)
O4W—Sm1—O11	69.01(10)	C22—N21—H21	118.5
O4W—Sm1—O11^{i}	69.01(10)	C26—N21—H21	118.5
O5W^{i}—Sm1—O2W	136.56(8)	C26—N21—C22	123.0(3)
O5W—Sm1—O2W	136.56(8)	C22—N23—H23	116.8
O5W^{i}—Sm1—O5W	83.80(17)	C24—N23—H23	116.8
O11—Sm1—O2W	66.37(8)	C24—N23—C22	126.3(3)
O11^{i}—Sm1—O2W	66.37(8)	O12—C12—N11	123.3(4)
O11—Sm1—O5W	71.55(10)	O12—C12—N13	122.5(4)
O11^{i}—Sm1—O5W^{i}	71.55(10)	N11—C12—N13	114.3(3)
O11^{i}—Sm1—O5W	138.82(10)	O14—C14—N13	119.2(4)
O11—Sm1—O5W^{i}	138.82(10)	O14—C14—C15	125.5(4)
O11—Sm1—O11^{i}	106.34(13)	N13—C14—C15	115.3(4)
O7W—Na1—O8W	95.9(3)	C14—C15—H15	120.1
O7W—Na1—O10W	85.2(3)	C16—C15—C14	119.8(4)
O7W—Na1—O12^{ii}	90.1(2)	C16—C15—H15	120.1
O7W—Na1—O22	101.5(2)	N11—C16—C17	115.9(3)
O8W—Na1—O10W	83.2(3)	C15—C16—N11	120.8(4)
O8W—Na1—O12^{ii}	145.7(3)	C15—C16—C17	123.2(4)
O8W—Na1—O22	63.8(2)	O13—C17—O11	126.8(4)
O10W—Na1—O22	146.6(3)	O13—C17—C16	116.1(4)
O12^{ii}—Na1—O10W	131.1(4)	O11—C17—C16	117.1(4)
O12^{ii}—Na1—O22	81.91(16)	O22—C22—N21	122.4(4)
O14—Na1—O7W	169.7(3)	O22—C22—N23	122.9(4)
O14—Na1—O8W	93.8(2)	N21—C22—N23	114.7(3)
O14—Na1—O10W	92.5(3)	O24—C24—N23	119.6(4)
O14—Na1—O12^{ii}	83.89(16)	O24—C24—C25	125.3(4)

O14—Na1—O22	85.94(17)	N23—C24—C25	115.1(4)
Sm1—O1W—H1W	127(4)	C24—C25—H25	120.0
Sm1—O1W—H1W^{i}	127(4)	C26—C25—C24	120.0(4)
H1W—O1W—H1W^{i}	104(7)	C26—C25—H25	120.0
Sm1—O2W—H2W	106(4)	N21—C26—C27	117.8(3)
Sm1—O2W—H2W^{i}	106(4)	C25—C26—N21	120.7(4)
H2W—O2W—H2W^{i}	108(7)	C25—C26—C27	121.4(4)
Sm1—O3W—H3WA	109(4)	O23—C27—O21	126.7(4)
Sm1—O3W—H3WB	133(4)	O23—C27—C26	117.6(4)
H3WA—O3W—H3WB	106(4)	O21—C27—C26	115.7(3)

Sm1—O11—C17—O13	13.3(7)	C14—N13—C12—O12	179.8(4)
Sm1—O11—C17—C16	−166.7(2)	C14—N13—C12—N11	−0.1(6)
Na1^{iii}—O12—C12—N11	19.9(7)	C14—C15—C16—N11	−0.5(6)
Na1^{iii}—O12—C12—N13	−160.0(3)	C14—C15—C16—C17	−179.2(4)
Na1—O14—C14—N13	154.3(3)	C15—C16—C17—O13	171.8(4)
Na1—O14—C14—C15	−25.4(7)	C15—C16—C17—O11	−8.2(6)
Na1—O22—C22—N21	89.3(4)	C16—N11—C12—O12	178.8(4)
Na1—O22—C22—N23	−91.3(4)	C16—N11—C12—N13	−1.3(6)
O14—C14—C15—C16	179.0(4)	C22—N21—C26—C25	2.3(6)
O24—C24—C25—C26	177.6(4)	C22—N21—C26—C27	−176.3(4)
N11—C16—C17—O13	−7.0(5)	C22—N23—C24—O24	−176.9(4)
N11—C16—C17—O11	173.0(3)	C22—N23—C24—C25	2.9(6)
N13—C14—C15—C16	−0.7(6)	C24—N23—C22—O22	179.4(4)
N21—C26—C27—O23	−1.6(6)	C24—N23—C22—N21	−1.1(6)
N21—C26—C27—O21	177.5(4)	C24—C25—C26—N21	−0.2(6)
N23—C24—C25—C26	−2.2(6)	C24—C25—C26—C27	178.3(4)
C12—N11—C16—C15	1.6(6)	C25—C26—C27—O23	179.9(4)
C12—N11—C16—C17	−179.6(4)	C25—C26—C27—O21	−1.1(6)
C12—N13—C14—O14	−178.7(4)	C26—N21—C22—O22	177.9(4)

C12—N13—C14—C15	1.0(6)	C26—N21—C22—N23	−1.6(5)

Symmetry codes: (i) −*x*, *y*, *z*; (ii) −*x*+1/2, *y*−1/2, *z*; (iii) −*x*+1/2, *y*+1/2, *z*.