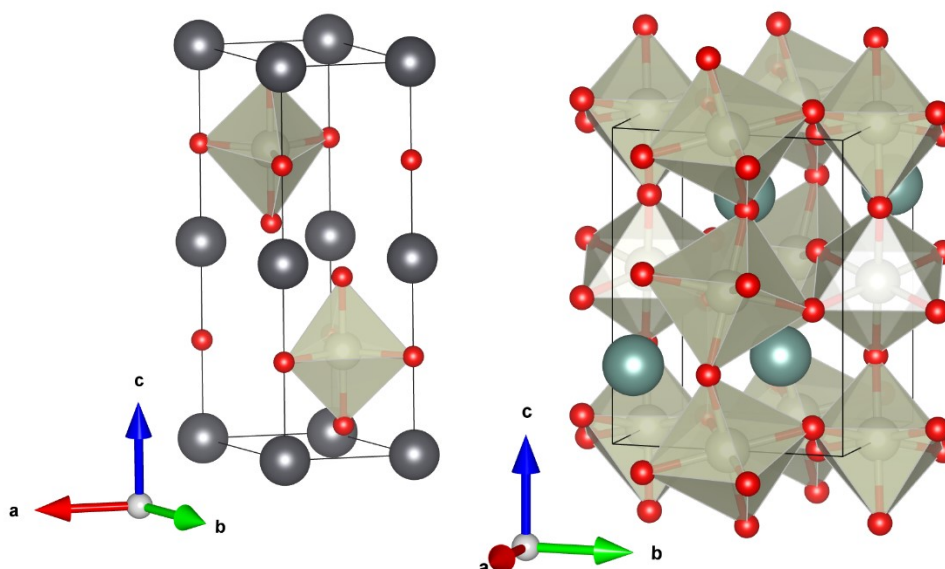


Figure SI1: TGA plots for Pb₂Rh₂O₇ and Y₂Rh₂O₇.

Table SI1

Material	PbRhO ₃	YRhO ₃
Space Group	<i>P6₃/mmc</i>	<i>Pbnm</i>
a (Å)	3.61190(3)	5.522708(20)
b (Å)	3.61190(3)	5.72375(23)
c (Å)	11.15743(15)	7.57282(25)
γ (°)	120	90
Volume (Å ³)	126.057(2)	226.568(15)
Pb/Y (x,y,z)	0, 0, 0	0.9787(21), 0.0844(15), ¼
Rh (x,y,z)	1/3, 2/3, 1/2	0 ½ 0
O1 (x,y,z)	0, 0, ¼	0.1215(30), 0.4541(25), ¼
O2 (x,y,z)	1/3, 2/3, 0.062(6)	0.6786(18), 0.3143(20), 0.0639(14)

Thermal displacement parameters were kept at nominal values ($B_{\text{iso}} = 1$) and not refined



Refined crystal structures for PbRhO₃ (left) and YRhO₃ (right)

Table S12

Composition	Pb ₂ Rh ₂ O ₇		Y ₂ Rh ₂ O ₇	
Space group	<i>Fd3m</i>		<i>Fd3m</i>	
Parameters	Experiment	Theory (GGA+U)	Experiment	Theory (GGA+U)
<i>a</i> (Å)	10.10568(2)	10.201	10.11834(5)	10.149
Volume (Å ³)	1032.146(4)	1061.439	1035.924(9)	1045.282
<i>A</i> (x,y,z) 16 <i>c</i>	½, ½, ½	½, ½, ½	½, ½, ½	½, ½, ½
Rh (x,y,z) 16 <i>d</i>	0, 0, 0	0, 0, 0	0, 0, 0	0, 0, 0
O1 (x,y,z,) 48 <i>f</i>	0.33607(15), 1/8, 1/8	0.33577, 1/8, 1/8	0.33536(17), 1/8, 1/8	0.335098, 1/8, 1/8
O2 (x,y,z) 8 <i>b</i>	3/8, 3/8, 3/8	3/8, 3/8, 3/8	3/8, 3/8, 3/8	3/8, 3/8, 3/8
A–O1 (Å)	2.4347(11)	2.4613	2.4443(12)	2.4534
A–O2 (Å)	2.1879	2.2085	2.1907	2.1972
Rh–O1 (Å)	1.9880(10)	2.0043	1.9863(11)	1.9911
Rh–O1–Rh (°)	127.8(3)	128.23	128.46(3)	128.58

CSD deposition numbers:

Pb₂Rh₂O₇: 2324706

Y₂Rh₂O₇: 2324707

PbRhO₃: 2324705