Electronic Supplementary Information (ESI)

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Table S1: The structure refinement data for RbHSH crystal

Theta range for data collection	2.73 to 28.28°	
Index ranges	-10<=h<=10, -10<=k<=10, -10<=l<=10	
Reflections collected	11924	
Independent reflections	2106 [R(int) = 0.0456]	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma w (F_o^2 - F_c^2)^2$	
Data/restraints/parameters	2106 / 0 / 118	
Goodness-of-fit on F^2	1.192	
Final R indices	1932 data; I>2σ(I)	R1 = 0.0335, wR2 = 0.0817
	all data	R1 = 0.0386, wR2 = 0.0842
Weighting scheme	$w=1/[\sigma^2(F_o^2) +(0.0445P)^2+0.0732P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.588 and -1.034 eÅ^{-3}	
R.M.S. deviation from the mean	0.199 eÅ^{-3}	

Table S2: Bond lengths (Å) of the grown crystal

Atoms	Bond length	Atoms	Bond length
Rb1-O2	2.827(2)	Rb1-O3#4	2.930(2)
Rb1-O4#6	2.955(2)	Rb1-O4#2	2.979(2)

Rb1-O6#3	2.995(2)	Rb1-O6#4	3.077(2)
Rb1-O7#1	3.090(2)	Rb1-C9#6	3.545(3)
Rb1-Rb1#6	4.3442(7)	Rb1-Rb1#5	4.4078(8)
O2-C8	1.260(3)	O4-C11	1.215(3)
O3-C8	1.247(3)	O7-C12	1.326(3)
O6-C12	1.209(3)	O5-C11	1.310(3)
O5-H5	0.820000	C8-C9	1.526(4)
C12-C13	1.511(4)	C11-C10	1.497(4)
C13-C13#7	1.508(5)	C13-H13A	0.970000
C13-H13B	0.970000	C9-C10	1.516(4)
C9-H9A	0.970000	C9-H9B	0.970000
C10-H10A	0.970000	C10-H10B	0.970000

Table.S3: Bond angles of the RbHSH crystal

Atoms	Bond angles	Atoms	Bond angles
O2-Rb1-O3#7	75.73(6)	O2-Rb1-O4#9	143.57(6)
O3#7-Rb1-O4#9	128.22(6)	O2-Rb1-O4#3	70.68(6)
O3#7-Rb1-O4#3	83.66(6)	O4#9-Rb1-O4#3	84.07(6)
O2-Rb1-O6#5	79.08(7)	O3#7-Rb1-O6#5	146.89(6)
O4#9-Rb1-O6#5	84.48(6)	O4#3-Rb1-O6#5	107.86(6)
O2-Rb1-O6#7	90.43(6)	O3#7-Rb1-O6#7	70.55(5)
O4#9-Rb1-O6#7	121.63(6)	O4#3-Rb1-O6#7	151.31(6)
O6#5-Rb1-O6#7	88.64(5)	O2-Rb1-O7#1	145.88(6)
O3#7-Rb1-O7#1	70.16(6)	O4#9-Rb1-O7#1	64.56(6)
O4#3-Rb1-O7#1	103.99(6)	O6#5-Rb1-O7#1	132.40(6)
O6#7-Rb1-O7#1	79.36(6)	O2-Rb1-C9#9	140.56(6)
O3#7-Rb1-C9#9	127.12(6)	O4#9-Rb1-C9#9	52.02(6)
O4#3-Rb1-C9#9	135.43(6)	O6#5-Rb1-C9#9	65.57(6)
O6#7-Rb1-C9#9	72.52(6)	O7#1-Rb1-C9#9	66.88(6)
O2-Rb1-Rb1#9	82.80(4)	O3#7-Rb1-Rb1#9	109.97(4)

O4#9-Rb1-Rb1#9	107.76(4)	O4#3-Rb1-Rb1#9	146.38(4)
O6#5-Rb1-Rb1#9	45.08(4)	O6#7-Rb1-Rb1#9	43.56(4)
O7#1-Rb1-Rb1#9	109.52(4)	C9#9-Rb1-Rb1#9	60.15(4)
O2-Rb1-Rb1#8	108.41(4)	O3#7-Rb1-Rb1#8	109.89(4)
O4#9-Rb1-Rb1#8	42.24(4)	O4#3-Rb1-Rb1#8	41.83(4)
O6#5-Rb1-Rb1#8	98.21(4)	O6#7-Rb1-Rb1#8	160.82(4)
O7#1-Rb1-Rb1#8	82.84(4)	C9#9-Rb1-Rb1#8	93.95(4)
Rb1#9-Rb1-Rb1#8	140.119(13)	C8-O2-Rb1	133.67(18)
C11-O4-Rb1#9	130.95(18)	C11-O4-Rb1#4	130.08(18)
Rb1#9-O4-Rb1#4	95.93(6)	C8-O3-Rb1#7	126.58(18)
C12-O7-Rb1#6	119.53(16)	C12-O6-Rb1#2	146.07(18)
C12-O6-Rb1#7	121.79(18)	Rb1#2-O6-Rb1#7	91.36(5)
C11-O5-H5	109.500000	O3-C8-O2	125.7(3)
O3-C8-C9	119.3(2)	O2-C8-C9	115.0(2)
O6-C12-O7	123.2(3)	O6-C12-C13	124.8(2)
O7-C12-C13	112.0(2)	O4-C11-O5	123.9(3)
O4-C11-C10	125.7(2)	O5-C11-C10	110.3(2)
C13#10-C13-C12	113.8(3)	C13#10-C13-H13A	108.800000
C12-C13-H13A	108.800000	C13#10-C13-H13B	108.800000
C12-C13-H13B	108.800000	H13A-C13-H13B	107.700000
C10-C9-C8	113.3(2)	C10-C9-Rb1#9	107.00(16)
C8-C9-Rb1#9	138.85(17)	C10-C9-H9A	108.900000
C8-C9-H9A	108.900000	Rb1#9-C9-H9A	47.500000
C10-C9-H9B	108.900000	C8-C9-H9B	108.900000
Rb1#9-C9-H9B	63.600000	H9A-C9-H9B	107.700000
C11-C10-C9	116.2(2)	C11-C10-H10A	108.200000
C9-C10-H10A	108.200000	C11-C10-H10B	108.200000
C9-C10-H10B	108.200000	H10A-C10-H10B	107.400000

Table.S4: Hydrogen bond distances (Å) and angles (°) of RbHSH crystal

	Donor-H	Acceptor-H	Donor-Acceptor	Angle
O5-H5...O2#1	0.82	1.72	2.528(3)	169.3
C10-H10B... O2#2	0.97	2.63	3.579(4)	166.1

Table.S5: Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for RbHSH.

	x/a	y/b	z/c	U(eq)
H5	0.7457	0.5159	1.1826	0.059000
H13A	1.0815	0.1441	-0.0325	0.026000
H13B	1.1713	-0.0587	0.0501	0.026000
H9A	0.7660	0.6998	0.6029	0.025000
H9B	0.5601	0.6620	0.7015	0.025000
H10A	0.7208	0.3801	0.8568	0.029000
H10B	0.9126	0.4434	0.7728	0.029000

Table.S6: lists the numerous functional groups present in the compound.

Wave numbers(cm^{-1})	Assignments
2932	CH_2 stretching vibration
2535	Atmospheric CO_2

1684	C=O stretching vibration
1415	symmetric stretching vibration of COO^-
1299	C-O-H bending vibration
1199-1178	C-O stretching vibration
1042	C=O bending vibration
804	C-H deformation
714-631	metal-oxygen vibration
471, and 561	presence of metal complexes

Table.S7: Mechanical parameters of the RbHSH crystal

Load P (gm)	H_v (Kg/mm^2)	C11 $\times 10^{14}$ Pa	σ_y (Kg/mm^2)
10	95.63415	2924.642	31.87805
20	85.02849	2380.882	28.34283
30	70.42997	1712.283	23.47666
50	61.24223	1340.723	20.41408
80	52.0346	1008.118	17.34487
90	42.76095	715.044	14.25365

Table.S8: Amplitude parameters of the grown RbHSH crystal measured by AFM

S.NO	Amplitude parameters	Value
1	Area Roughness	618 pm^2
2	Roughness average (S_a)	97.076nm

3	Root mean square (S_q)	160.24nm
4	Peak-valley height (S_y)	2044.6nm
5	Peak height (S_p)	844.51nm
6	Valley depth (S_v)	-1200.1nm
7	The mean value (S_m)	-10.014pm
8	Image size	25μm