

Table S1 Selected bond and hydrogen bond distances and angles for potassium glycolate glycolic acid

	distance (Å)		angle (°)
K-O1	2.826(1)		
	2.913(1)		
K-O2	3.086(1)		
K-O3	2.893(2)		
	3.074(2)		
K-O5	2.834(1)		
	2.838(1)		
	2.883(1)		
K-O6	2.780(1)		
average	2.903		
C1-O1	1.268(1)	<O1-C1-O2	123.09(13)
C1-O2	1.241(2)	<O1-C1-C2	116.28(13)
C1-C2	1.516(3)	<O2-C1-C2	120.62(14)
C2-H2A	0.96(3)		
C2-H2B	0.93(3)		
C2-O3	1.409(3)	<O3-C2-C1	111.98(13)
O3-H3	0.83(3)		
O4-H4	0.86(3)		
C3-O4	1.307(2)	<O4-C3-O5	124.11(14)
C3-O5	1.218(2)	<O4-C3-C4	111.86(13)
C3-C4	1.506(3)	<O5-C3-C4	124.03(14)
C4-H4A	0.96(2)		
C4-H4B	0.92(3)		
C4-O6	1.404(3)	<O6-C4-C3	113.17(13)
O6-H6	0.83(3)		
O3-H3...O2	1.91(3)	<O3-H3...O2	170(3)
O3...O2	2.733(2)		
O4-H4...O1	1.66(3)	<O4-H4...O1	176(4)
O4...O1	2.519(2)		
O6-H6...O2	1.94(3)	<O6-H6...O2	163(3)
O6...O2	2.745(2)		

Table S2 Assignments of major vibrational bands for potassium glycolate hemihydrate and potassium glycolate glycolic acid based on experimental results.

Assignment	K(C ₂ H ₃ O ₃)·H ₂ O		K(C ₂ H ₃ O ₃)(C ₂ H ₄ O ₃)	
	FTIR (cm ⁻¹)	Raman (cm ⁻¹)	FTIR (cm ⁻¹)	Raman (cm ⁻¹)
$\nu_{as}H_2O$	3298			
$\nu O-H$	3234/3168		3296/3223	
ν_sCH_2	2956/2904		2953/2924	
$O-H\cdots O$	2800-2300			
$\nu O-H$ in - COOH			2545/2490/2441	
δH_2O	1629	1613		
$\nu_{as}COO^-$ ($\nu_{as}COOH$) + ωCH_2	1699/1593	1695/1577	1703/1599/1577	
$\beta O-H$ + ν_sCOO^- ($\nu_{as}COOH$) + $\nu C-C$ + ωCH_2 + δCH_2	1469/1442/1398/1378/1 302	1469/1439/1387/13 04	1469/1433/1419/1400/1 386	1468/1431/1418/13 86
$\beta O-H$ + τCH_2 τCH_2	1280	1278 1249	1294/1267/1246	1287/1251
$\nu C-OH$	1080	1082	1095	1106
ρCH_2	1016/995		1012	
$\nu C-C$	933/920	918	995/933	995/935
τH_2O + $\gamma O-H$ ωH_2O + $\gamma O-H$ $\gamma O-H$	790 744		681	680
ρH_2O	700/669	668		
$\delta HO-CH_2-$ COO^- + $\nu K-O$	<600	<600	<600	<600

ν : stretching vibration, ν_{as} : asymmetric stretching vibration, ν_s : symmetric stretching vibration, β : in plane vibration, γ : out of plane vibration, δ : scissoring vibration in plane, ρ : rocking vibration in plane, ω : angular deformation out of plane, τ : twisting vibration out of plane.

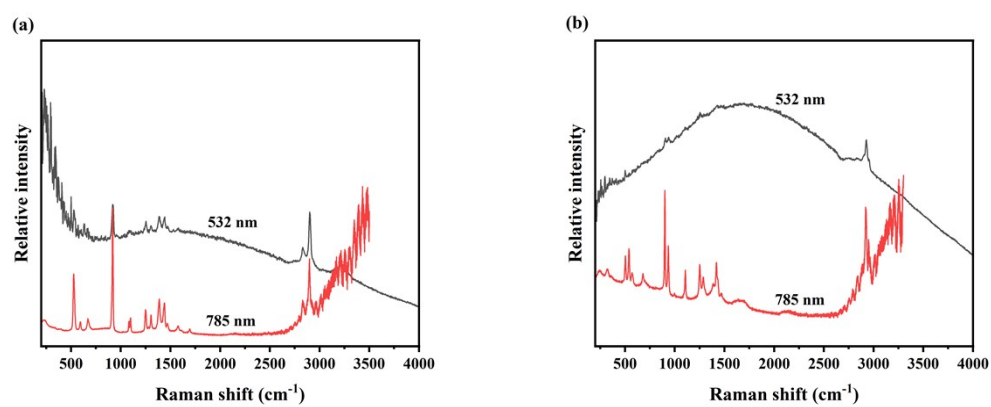


Fig. S1 Raman spectra: (a) Raman spectra of potassium glycolate hemihydrate; (b) Raman spectra of potassium glycolate glycolic acid.
