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NOTE

Hydrothermal Synthesis and Crystal Structure of Sodium(2S)-2-amino-5-hydroxy-5-oxo-pentanoate

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One new sodium glutamate *i.e.*, sodium(2S)-2-amino-5-hydroxy-5-oxo-pentanoate has been successfully synthesized. The compound has been characterized by X-ray single-crystal diffraction, Compound shows a one-dimensional framework. The 3D supramolecular structure is formed *via* hydrogen bonding connection.

Keywords: Coordination polymer, Crystal structure, Sodium.

Metal organic frameworks (MOFs) have received much attention in the field of crystal engineering and supramolecular chemistry because of their diverse structures and promising applications in functional materials such as luminescent materials, gas adsorption and magnetism[1-4]. Hydrogen bonds are well suited for the design of polymeric arrangement and crystal engineering because of their important directional interactions and because they can interlink 1-D, or 3-D structures into higher-dimensionality systems[5,6]. In present work, the hydrothermal synthesis and crystal structure of sodium(2S)-2-amino-5-hydroxy-5-oxo-pentanoate are reported.

All the reagent and solvents employed were commercially available and used as received without further purification.

General procedure: Sodium glutamate (0.5 mmol) issolved in distilled water (20 mL) and stirred for 2 h at room temperature and the result liquid was kept at room temperature and filtered. The obtained solid was washed by deionized water and dried. Then the colourless block-shaped crystals were obtained.

Diffraction intensity data of the single crystal of the five compounds were collected on a Bruker SMART APEXII CCD diffractometer equipped with a graphite monochromated MoK_α radiation ($\lambda = 0.71073$ Å) by using a ω-scan mode. All the structures were solved by direct methods and refined by full-matrix least-squares methods on F^2 using the program SHEXL 97[7]. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were located by geometrically calculations and their positions and thermal parameters were fixed during the structure refinement. The crystallographic data and experimental details of structural analyses for coordination polymers are summarized in Table-1. Selected bond and angle parameters are listed in Table-2. CCDC: 978565.

X-ray diffraction analysis revealed that the fundamental building unit consists of the sodium atom and amino acid. The bond connecting the sodium atom and oxygen atom is a single bond, which can rotate and this is confirmed by the bond length of Na(1)-O(1), Na(1)-O(5), Na(1)-O(9) are 2.4408(16),

TABLE-1
CRYSTALLOGRAPHIC DATA AND STRUCTURE REFINEMENT SUMMARY FOR COMPLEX

Empirical formula	$C_{10}H_{20}N_2O_{10}Na_2$	Z, Calculated density (mg/m^3)	4, 1.635
Formula weight	374.26	Absorption coefficient (mm^{-1})	0.190
Crystal system space group	Orthorhombic, P2(1)2(1)2(1)	F(000)	784
Unit cell dimensions	a = 5.5606(11) Å b = 15.235(3) Å c = 17.949(4) Å	Limiting indices	-6 ≤ h ≤ 6 -18 ≤ k ≤ 18 -21 ≤ l ≤ 21
Volume (Å^3)	1520.5(5)	Largest diff. peak and hole (e/Å^3)	0.171 and 0.171
θ range for data collection	2.63 -25.50	Goodness-of-fit on F^2	1.033
Final R indices [I >2σ(I)]	$R_1 = 0.0292$, $wR_2 = 0.0700$	R indices (all data)	$R_1 = 0.0348$, $wR_2 = 0.0729$

TABLE –2
SELECTED BOND LENGTHS (Å) AND ANGLES(°) FOR COMPLEX

Na(1)-O(2)#1	2.3082(16)	Na(1)-O(5)	2.4429(17)
Na(1)-O(9)	2.3987(17)	Na(1)-O(10)	2.5481(18)
Na(1)-O(1)	2.4408(16)	Na(1)-O(8)#2	2.4036(16)
Na(2)-O(1)	2.3608(15)	Na(2)-O(9)	2.5770(18)
Na(2)-O(2)	2.4621(16)	Na(2)-O(6)#5	2.3929(16)
O(9)-Na(1)-O(1)	77.69(5)	O(2)#1-Na(1)-O(8)#2	100.36(6)
O(9)-Na(1)-O(5)	108.49(6)	O(9)-Na(1)-O(8)#2	88.10(6)
O(1)-Na(1)-O(5)	97.88(5)	O(2)#1-Na(1)-O(1)	94.02(6)
O(9)-Na(1)-O(10)	82.81(6)	O(8)#2-Na(1)-O(1)	165.60(6)
O(2)#1-Na(1)-O(10)	86.05(6)	O(4)#3-Na(2)-O(1)	120.24(6)
O(8)#2-Na(1)-O(10)	83.67(6)	O(10)#4-Na(2)-O(1)	141.58(6)

Symmetry codes: #1 x-1, y, z ; #2 x-1/2, -y + 1/2, -z + 1; #3 –x + 1/2, -y, z-1

2.4429(17), 2.3987(17) Å. In addition, inspection reveals that there are several obvious hydrogen bond interactions between the adjacent units mentioned above involving to the ammonium cation, the carboxylic and the carboxylate group as well as the water molecule (Fig. 1). Some are listed as follows: N(1)-H(1A)...O(4)#10, [N...O = 2.871(2) Å, N--H...O = 174.6 Å]; N(1)-H(1B)...O(5)#4, [O...N = 3.002(2) Å, N--H...O = 161.8°]; N(1)-H(1C)...O(3)#4, [O...N = 2.809(2) Å, N--H...O = 161.6°]; N(2)-H(2A)...O(7)#1, [N...O = 2.770(2) Å, N--H...O = 167.3°]; N(2)-H(2B)...O(6)#1, [O...N = 2.919(2) Å, N--H...O = 162.3 °];N(2)-H(2C)...O(8)#2, [O...N = 2.943(2) Å, N--H...O = 165.9°];O(9)-H(1W)...O(8)#8, [O...O = 2.836(2) Å, O--H...O = 166.7°];O(9)-H(2W)...O(7)#2, [O...O = 2.787(2) Å, O--H...O = 168.3°];O(10)-H(3W)...O(4)#3, [O...O = 2.842(2) Å, O--H...O = 167.3°];O(10)-H(4W)...O(3)#9, [O...O = 2.828(2) Å, O--H...O = 174.4°]. Symmetry codes: #1 x-1, y, z; #2 x-1/2, -y + 1/2, -z + 1; #3 -x + 1/2, -y, z-1/2; #4 x + 1, y, z; #5 -x + 1, y-1/2, -z + 3/2; #6 -x + 1/2, -y, z + 1/2; #7 -x + 1, y + 1/2, -z + 3/2; #8 x + 1/2, -y + 1/2, -z + 1; #9 -x-1/2, -y, z-1/2 ; #10 x + 1/2, -y + 1/2, -z + 2.

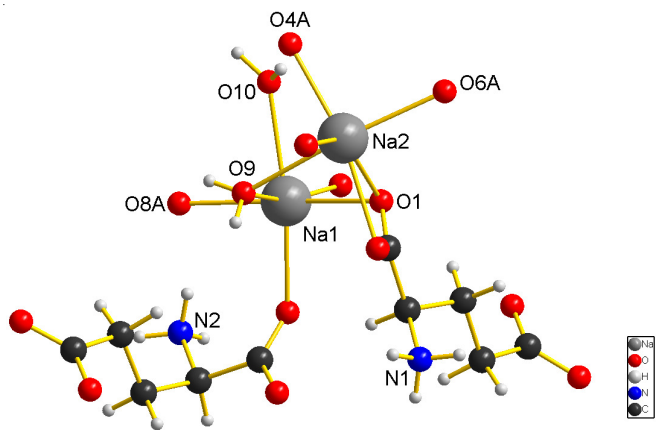

Fig. 1. Molecular structure of the title compound at 30 % probability displacement ellipsoids

The chains are further assembled by the intermolecular hydrogen bonding interaction leading to the formation of a 3D framework (Fig.2).

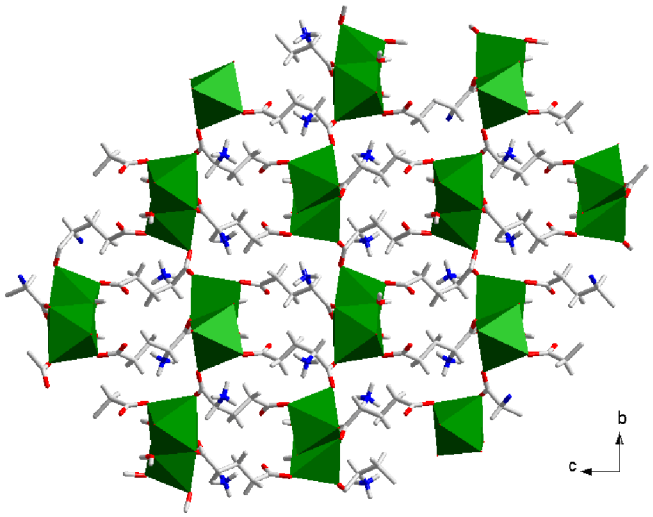

Fig. 2. 3D structure formed *via* hydrogen bonding interactions

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