Instrumental Achievements
—— X-Ray Analysis ——

Crystal and Molecular Structures of Monosodium L-Glutamate Monohydrate

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Monosodium L-glutamate crystallizes as a monohydrate from an aqueous solution at room temperature (Fig. 1). A crystal structure analysis of this crystal was reported by Rao *et al.*[1] at a congress, though no paper has yet been published. For the purpose of studying the crystal habit in the presence of other amino acids or organic acid contaminants, we have determined the structure of this crystal.

Monosodium L-glutamate monohydrate crystallizes as rhombic prisms and has an overgowth tendency to form polycrystals. Suitable crystals for an X-ray diffraction study were selected by the polarization microscope and ω-scan profile. Hydrogen atoms were found in a difference electron-density map, and were located at the calculated positions and were refined with isotopic temperature factors.

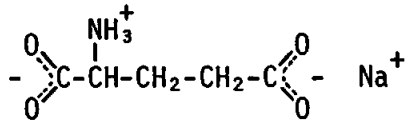

Fig. 1 Chemical structure.

Table 1 Crystal and experimental data

Compound name: Monosodium L-glutamate monohydrate
Formula: $C_5H_8NO_4 \cdot Na \cdot H_2O$
Formula weight: 187.13
Crystal system: Orthorhombic
Space group: $P2_12_12_1$ $Z=8$
a=15.237(8) Å,
b=17.937(9) Å,
c=5.562(4) Å,
V=1520 Å^3
D_x=1.635 g cm^{-3}, D_m=1.63 g cm^{-3}
R=0.037
No. of reflections used=1805
Measurement: Philips PW1100
Program system: Private
Structure determination: MULTAN
Refinement: Block-diagonal

Glutamic acid molecules are zwitterion form, as shown in Fig. 2 (also showing molecular conformations).

The conformations of the two molecules in an asymmetric unit are different, as shown in Table 3. Remarkable differences between them appear in the torsion angles of chi 1 and chi 3.

Both Na ions are coordinated in octahedra with four (3 alpha and 1 gamma) carboxyl oxygen atoms, and two water molecules. These coordination polyhedra are

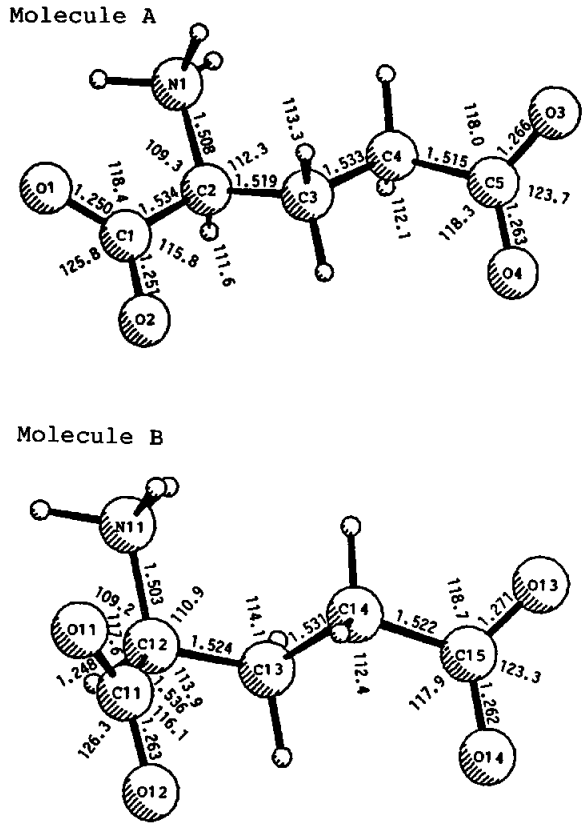

Fig. 2 Molecular conformations with bond lengths and angles.

Table 2 Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic thermal parameters ($\times 10^2$) (with e.s.d.'s in parentheses) $B_{eq}=(4/3)\Sigma_i\Sigma_j\beta_{ij}\boldsymbol{a}_i\boldsymbol{a}_j$

	x	y	z	$B_{eq}/Å^2$
Molecule A				
C1	5560(2)	2186(2)	5161(6)	144(4)
C2	6305(2)	1633(2)	4646(6)	140(4)
C3	5979(2)	959(2)	3252(7)	166(4)
C4	6712(2)	412(2)	2580(7)	184(4)
C5	6411(2)	-162(2)	757(6)	150(4)
N1	6740(2)	1418(1)	6980(5)	163(4)
O1	5486(1)	2440(1)	7245(4)	189(3)
O2	5092(1)	2359(1)	3398(4)	181(3)
O3	6521(1)	-844(1)	1255(5)	181(3)
O4	6086(2)	68(1)	-1196(5)	219(3)
Molecule B				
C11	7921(2)	2794(2)	1487(6)	155(4)
C12	8600(2)	3274(2)	157(6)	147(4)
C13	8948(2)	3926(2)	1633(7)	168(4)
C14	8225(2)	4513(2)	2252(7)	179(4)
C15	8589(2)	5087(2)	4045(6)	158(4)
N11	8211(2)	3542(2)	-2172(5)	180(4)
O11	7226(1)	2640(1)	409(5)	208(3)
O12	8128(1)	2589(1)	3585(4)	192(3)
O13	8521(2)	5770(1)	3532(5)	191(3)
O14	8905(2)	4852(1)	6020(5)	210(3)
Water and Ions				
O(W1)	9369(2)	1111(1)	661(5)	270(4)
O(W2)	5658(2)	3966(1)	4024(5)	272(4)
Na1	5769(1)	3204(1)	499(3)	179(2)
Na2	9317(1)	1748(1)	4328(3)	188(2)
Coordinates of hydrogen atoms ($\times 10^3$) and Beq				
H(C2)	680(3)	192(2)	357(9)	4.6 (1.2)
H(C3)1	566(3)	114(2)	161(9)	4.9 (1.2)
H(C3)2	549(3)	66(2)	434(9)	4.6 (1.1)
H(C4)1	694(3)	12(3)	418(10)	5.4 (1.3)
H(C4)2	727(3)	72(2)	181(9)	4.5 (1.1)
H(N1)1	638(3)	96(3)	782(10)	6.0 (1.4)
H(N1)2	675(3)	189(3)	818(10)	6.8 (1.5)
H(N1)3	741(3)	124(3)	666(10)	5.4 (1.3)
H(C12)	914(3)	290(2)	-29(9)	4.4 (1.1)
H(C13)1	947(3)	421(2)	65(9)	4.4 (1.1)
H(C13)2	922(3)	372(2)	331(9)	4.2 (1.1)
H(C14)1	768(3)	424(2)	304(9)	4.1 (1.1)
H(C14)2	805(3)	480(3)	64(10)	5.6 (1.3)
H(N11)1	823(3)	310(3)	-349(10)	6.5 (1.4)
H(N11)2	859(3)	401(3)	-284(10)	5.6 (1.2)
H(N11)3	754(3)	372(3)	-190(10)	5.7 (1.3)
H(OW1)1	926(3)	68(3)	153(10)	5.9 (1.3)
H(OW1)2	900(3)	107(2)	-43(9)	5.2 (1.2)
H(OW2)1	565(3)	437(3)	346(9)	5.5 (1.2)
H(OW2)2	597(3)	399(2)	544(9)	5.3 (1.2)

Table 3 Torsion angles (°) with e.s.d.'s

		Molecule A	Molecule B
psi 1	O1-C-Cα-N	8.2(3)	6.9(3)
psi 2	O2-C-Cα-N	-173.8(1)	-173.4(1)
chi 1	N-Cα-Cβ-Cγ	-60.0(3)	58.7(3)
chi 2	Cα-Cβ-Cγ-Cδ	-167.7(2)	170.9(2)
chi 31	Cβ-Cγ-Cδ-O3	-126.5(2)	127.2(2)
chi 32	Cβ-Cγ-Cδ-O4	55.5(3)	-54.6(3)

Table 4 Na–O distances (Å) (with e.d.s.'s), in MSG crystal

Na1	O1	x,y,-1+z	2.311(3)
	O2	x,y,z	2.442(3)
	O11	x,y,z	2.440(3)
	O13	1+1/2-x,1-y,-1/2+z	2.400(3)
	O(W1)	-1/2,1/2-y,-z	2.545(3)
	O(W2)	x,y,z	2.396(3)
Na2	O1	1/2+x,1/2-y,1-z	2.461(3)
	O2	1/2+x,1/2-y,1-z	2.358(3)
	O3	1+1/2-x,-y,1/2+z	2.326(3)
	O12	x,y,z	2.394(3)
	O(W1)	x,y,z	2.339(3)
	O(W2)	1/2+x,1/2-y,1-z	2.579(3)

linked together by sharing the edges and are elongated along the *c* axis.

Reference

1. S. T. Rao and M. Mallikarjunan, *10th Int'l Congress of Crystallography Collected Abstracts,* 7-15 August, p. S48, 03.5 - 5 (1975), Amsterdam.

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