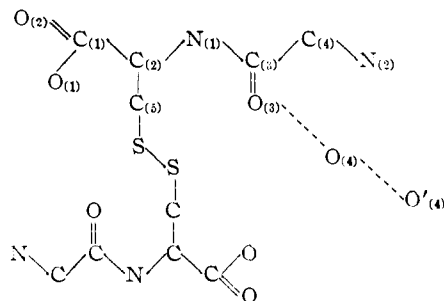


coordinates are given in the following tables. The numbering scheme used to identify the atoms in the asymmetric unit should be clear from the accompanying sketch.



BOND LENGTHS IN *N,N'*-DIGLYCYL-L-CYSTINE DIHYDRATE

Bond	R_{ij} Å.	Hydrogen bond	R_{ij} Å.
S-S	2.04	N ₁ -O ₃	3.31
S-C ₅	1.86	N ₂ -O ₁	2.75
C ₅ -C ₂	1.52	N ₂ -O ₁ '	2.89
C ₅ -C ₁	1.55	N ₂ -O ₂	2.75
C ₁ -O ₁	1.24	O ₄ -O ₄ '	2.91
C ₁ -O ₂	1.21	O ₄ -O ₃	3.13
C ₂ -N ₁	1.48		
N ₁ -C ₃	1.35	Average probable error in distances is 0.02 Å.	
C ₃ -O ₃	1.21	O ₄ refers to the oxygen atom of the water of hydration.	
C ₃ -C ₄	1.55		
C ₄ -N ₂	1.46		

BOND ANGLES IN *N,N'*-DIGLYCYL-L-CYSTINE DIHYDRATE

Angle	θ_i degrees	Hydrogen bond angle	θ_i degrees
S-S-C ₅	103	C ₄ -N ₂ -O ₁ '	85
S-C ₅ -C ₂	105	C ₄ -N ₂ -O ₁	129
C ₅ -C ₂ -C ₁	117	C ₄ -N ₂ -O ₂	112
C ₅ -C ₂ -N ₁	118	C ₁ -O ₁ -N ₂	143
C ₁ -C ₂ -N ₁	109	C ₁ -O ₁ -N ₂ '	96
O ₁ -C ₁ -O ₂	127	C ₁ -O ₂ -N ₂	126
C ₂ -C ₁ -O ₁	115	C ₃ -O ₃ -N ₁	144
C ₂ -C ₁ -O ₂	118	C ₂ -N ₁ -O ₃	140
C ₂ -N ₁ -C ₃	122	C ₃ -N ₁ -O ₃	96
N ₁ -C ₃ -O ₃	125	C ₃ -O ₃ -O ₄	106
C ₄ -C ₃ -O ₃	121	O ₃ -O ₄ -O ₄ '	118
N ₁ -C ₃ -C ₄	113	Average probable error in angles is 1°	
C ₃ -C ₄ -N ₂	109		

One of the many interesting features of this structure is the long hydrogen bond (3.31 Å.) existing between the respective amide groups of molecules related by the *b* repeat. Van der Waals repulsions between the molecules involved seem to be responsible for the unusual length. This weak bond is accompanied by a slight non-planarity of the amide group of the molecule. The non-planarity, which corresponds to a rotation of approximately 6° about the N₁-C₃ bond, introduces a strain energy calculated to be only 0.4 kcal./mole, however. The slightly long N₁-C₃ bond and the short C₃-O₃ bond may also be a consequence of the weak N₁-O₃ hydrogen bond.

The disposition of hydrogen bonds about the terminal nitrogen atom leaves no doubt concerning the zwitterion nature of this peptide. It may also be mentioned that the C₅-S-S-C₅' dihedral angle is calculated to be in 101° in good agreement

with the value found in S₈.² A more complete description of this investigation will appear shortly.

The authors wish to thank Dr. E. J. Cohn of Harvard University who kindly made available a sample of *N,N'*-diglycyl-L-cystine for this work.

(2) B. E. Warren and J. T. Burwell, *J. Chem. Phys.*, **3**, 6 (1935).

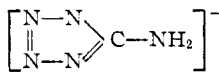
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NEW COMPOUNDS

Salts of 5-Aminotetrazole

The salts listed in Table I were prepared by either of two methods: (1) Equivalent quantities of anhydrous 5-aminotetrazole and the appropriate anhydrous amine or free guanidine base were caused to react in a minimum volume of hot, absolute methanol or ethanol; if the product did not crystallize upon cooling, a small volume of diethyl ether was added. (2) Equivalent quantities of 5-aminotetrazole monohydrate and the appropriate carbonate or bicarbonate salt of the base were dissolved in a small volume of water; the solution was evaporated to dryness to give the salt. These salts were recrystallized from absolute methanol, ethanol or mixtures of ethanol and diethyl ether. All of these salts were very soluble in water and in general were also appreciably soluble in methanol or ethanol. Salts derived from very volatile bases were unstable and readily dissociated into the free base and a residue of 5-aminotetrazole. For example, methylamine could be completely removed from its salt by heating at 80 to 100° for a few hours or by evacuating continuously at room temperature for a few days. For this reason the melting points of some of these salts were rather indefinite even when the sample was sealed in a capillary.

TABLE I

SALTS OF 5-AMINOTETRAZOLE [RH] ⁺ 			
R	Formula	M.p., °C. ^a	Nitrogen, % Calcd. Found
Hydrazine ^c	CH ₇ N ₇	124-125	^d ^d
Methylamine	C ₂ H ₉ N ₆	^e	72.38 72.51
Diethylamine	C ₅ H ₁₄ N ₆	^f	53.13 53.23
Ethylenediamine	C ₄ H ₁₄ N ₁₂	166-167	73.01 74.23
Piperidine	C ₆ H ₁₄ N ₆	176-178	49.38 49.43
Morpholine	C ₅ H ₁₂ N ₆	126-127	48.81 48.81
Benzylamine	C ₈ H ₁₂ N ₆	130.5-131.5	43.72 43.71
Guanidine	C ₂ H ₅ N ₅	126-126.5	77.74 78.45
Methylguanidine	C ₃ H ₁₀ N ₅	109-110	70.85 70.22
Phenylguanidine	C ₈ H ₁₂ N ₅	121-121.5	50.89 50.84
Aminoguanidine	C ₂ H ₉ N ₅	93-95	79.21 79.10
Benzalaminoguanidine	C ₉ H ₁₃ N ₅	145.5-146.5	50.99 51.09

^a The melting points are corrected. ^b Analyses by Margaret M. Mayfield. ^c This salt was first prepared by Howard W. Kruse, Inorganic Chemistry Branch, Chemistry Division, U. S. Naval Ordnance Test Station. ^d Calcd.: C, 10.25; H, 6.03. Found: C, 10.52; H, 6.17. ^e Melts 112-117° with preliminary softening from about 95°. ^f Melts 114-118° with preliminary softening from about 100°.

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