Such a hydrogen-bonding scheme is compatible with a specific interaction between arginine and guanine in DNA, with O(6) and N(7) of guanine replacing the waters bound to the terminal NH_2 groups. Helene (1977) has proposed such a scheme for the specific recognition of a G.C base pair by arginylglutamic acid.

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Structure of DL-α-Methyl-*m*-tyrosine (MMT), $C_{10}H_{13}NO_3$

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Abstract. $M_r = 195{\cdot}21$, monoclinic, $P2_1/c$, $a = 5{\cdot}933\,(1)$, $b = 9{\cdot}925\,(1)$, $c = 16{\cdot}679\,(2)$ Å, $\beta = 90{\cdot}71\,(1)°$, $V = 982{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}32$, $D_m = 1{\cdot}31$ Mg m^{-3}, $\mu = 6{\cdot}22$ mm^{-1}, $\lambda = 1{\cdot}5418$ Å, Cu $K\alpha$, $T = 291$ K, $F(000) = 416$, $R = 0{\cdot}048$ for 1438 unique reflections. The zwitterion forms an extended structure with torsional angles O—C′—C$^\alpha$—N [O(1)—C(1)—C(2)—N] $\psi = 5{\cdot}2\,(2)$, N—C$^\alpha$—C$^\beta$—C$^\gamma$ [N—C(2)—C(4)—C(5)] $\chi^1 = 301{\cdot}9\,(2)$, and C$^\alpha$—C$^\beta$—C$^\gamma$—C$^\delta$ [C(2)—C(4)—C(5)—C(6)] $\chi^2 = -93{\cdot}4\,(2)°$. The structure is stabilized by hydrogen bonding.

Introduction. The modified amino acid α-methyl-*m*-tyrosine (MMT) was one of the first analogues of tyrosine to be discovered as a precursor of a false neurochemical transmitter for sympathetic nerves. MMT acts as a substrate for the enzymes of norepinephrine biosynthesis, leading to the norepinephrine analogue metraminol (Kopin, 1971). This product accumulates in nerve endings in the same manner as normal transmitters of nerve impluses. However, their release upon stimulation leads to diminished nerve response and thus have been found useful as drugs for the relief of hypertension in man (Horita, 1971). It is of interest to understand the role of α-methylation on the conformation of this amino acid.

Experimental. Source, Sigma Chemical Co.; D_m by flotation in heptane–chloroform; plates, $0{\cdot}12 \times 0{\cdot}28 \times 0{\cdot}28$ mm; Picker FACS-I diffractometer; lattice parameters from 12 general reflections with $40° \leq 2\theta \leq 60°$; systematic absences, $h0l$, $l = 2n + 1$, $0k0$, $k = 2n + 1$; no absorption correction; $2\theta_{\max} = 128°$; range, $+h$, $+k$, $\pm l$; standard reflections, $14\bar{1}$, 152, 034 with standard deviation of 1·6%; 1818 measured, 1438 unique, 1018 observed at $3{\cdot}0\sigma(F)$ and $F \leq 12{\cdot}0$; $R_{\rm sym} = \sum\sum\big||F_i| - |\bar{F}_i|\big|/\sum\sum|\bar{F}_i| = 0{\cdot}01$; solved by direct methods (Long, 1965); based on F; H atoms located from difference Fourier, not refined; positional and anisotropic thermal parameters for nonhydrogen atoms refined; final R for unique $= 0{\cdot}048$, weighted $R = 0{\cdot}048$, $S = 1{\cdot}11$; weight evaluated from an analysis of $|\Delta F|$ *vs* F_o; $(\Delta/\sigma)_{\max} = 0{\cdot}16$, $(\Delta/\sigma)_{\rm av} = 0{\cdot}02$; min. height $\Delta F = -0{\cdot}06$, max. $= 0{\cdot}15$ e Å^{-3}; atomic scattering factors: nonhydrogen Cromer & Waber (1965), H Stewart, Davidson & Simpson (1965); computer programs in-house.

Discussion. The molecule is shown in Fig. 1 and the positional parameters are given in Table 1.* The bond lengths (Table 2) show no noticeable changes from those of L-tyrosine (Mostad, Nissen & Rømming, 1972)

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares-planes' data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38765 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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or α-methyl-*p*-tyrosine (MPT) (Gaudestad, Mostad & Rømming, 1976). The bond angles (Table 2) at the atom C^{α} reveal changes from tyrosine expected from the presence of the methyl group. The remaining bond angles are comparable to those of MPT. The angle at the C^{β} atom is significantly larger than the average value of 113·3° found in a survey of tyrosine compounds (Satyshur, 1978).

The deviation of the N atom from the plane of the carboxylate group in MMT and MPT is 0·114 and 0·035 Å respectively and may be due to the presence of the bulky methyl group. Much larger deviations can be expected and are found in unmethylated tyrosine structures (Cody, Duax & Hauptman, 1973). The angle χ^1 in L-MMT is *gauche*⁻ while it is *gauche*⁺ in L-MPT. Potential-energy calculations indicate a sharpening of the conformational domains for χ^1 and χ^2 rotations due to the presence of the methyl group (Satyshur, 1978).

The structure is stabilized by the presence of four hydrogen bonds (Fig. 2). The tyrosine base planes are not stacked but form a herring-bone pattern.

Table 1. *Positional parameters* (×10⁴) *for MMT*

Atom designation is in accordance with the IUPAC–IUB Commission on Biochemical Nomenclature (1970). Standard deviations are given in parentheses and refer to the least significant digit.

$$B_{eq} = \tfrac{4}{3}\textstyle\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq} (Å²)
O(1)	7346 (3)	−1427 (2)	5297 (1)	4·09 (6)
O(2)	9202 (3)	−2434 (2)	4307 (1)	3·28 (5)
O(3)	1376 (3)	−3371 (2)	1078 (1)	3·29 (5)
N	3422 (3)	−1435 (2)	4542 (1)	2·65 (6)
C(1) (C′)	7484 (4)	−1980 (2)	4616 (1)	2·63 (6)
C(2) (C^{α})	5292 (3)	−2128 (2)	4114 (1)	2·33 (6)
C(3)	4681 (5)	−3615 (3)	4043 (2)	3·28 (7)
C(4) (C^{β})	5679 (4)	−1436 (3)	3300 (1)	2·67 (6)
C(5) (C^{γ})	3688 (3)	−1382 (2)	2729 (1)	2·38 (6)
C(6) ($C^{\delta1}$)	3386 (4)	−2380 (3)	2153 (1)	2·58 (6)
C(7)	1567 (3)	−2341 (2)	1622 (1)	2·45 (6)
C(8)	45 (4)	−1287 (3)	1647 (1)	3·16 (6)
C(9)	359 (4)	−284 (3)	2214 (1)	3·38 (7)
C(10) ($C^{\delta2}$)	2147 (4)	−330 (3)	2753 (1)	2·89 (6)

Table 2. *Bond lengths* (Å) *and bond angles* (°) *for MMT*

Average standard deviation in the bond lengths is 0·004 Å and in bond angles 0·3°.

C(1)–O(1)	1·265	C(1)–O(2)	1·233	C(1)–C(2)	1·545
C(2)–N	1·494	C(2)–C(3)	1·524	C(2)–C(4)	1·541
C(4)–C(5)	1·509	C(5)–C(6)	1·390	C(6)–C(7)	1·388
C(7)–O(3)	1·371	C(7)–C(8)	1·383	C(8)–C(9)	1·384
C(9)–C(10)	1·383	C(10)–C(5)	1·389		

O(1)–C(1)–O(2)	126·6	C(4)–C(5)–C(6)	120·3
O(1)–C(1)–C(2)	117·7	C(4)–C(5)–C(10)	121·3
O(2)–C(1)–C(2)	115·7	C(5)–C(6)–C(7)	120·9
C(1)–C(2)–N	108·8	C(6)–C(7)–O(3)	117·3
C(1)–C(2)–C(3)	109·4	O(3)–C(7)–C(8)	122·4
C(1)–C(2)–C(4)	107·5	C(6)–C(7)–C(8)	120·3
N–C(2)–C(4)	109·6	C(7)–C(8)–C(9)	118·8
C(3)–C(2)–C(4)	113·6	C(8)–C(9)–C(10)	121·1
N–C(2)–C(3)	107·8	C(9)–C(10)–C(5)	120·4
C(2)–C(4)–C(5)	116·6	C(10)–C(5)–C(6)	118·5

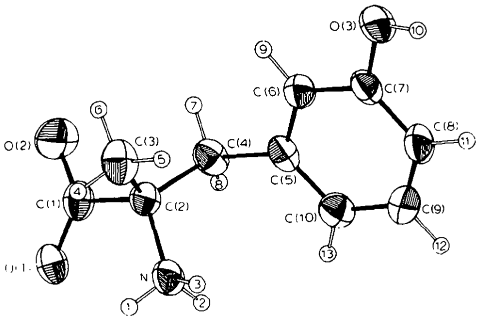

Fig. 1. An *ORTEP* (Johnson, 1965) plot of the molecule showing the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

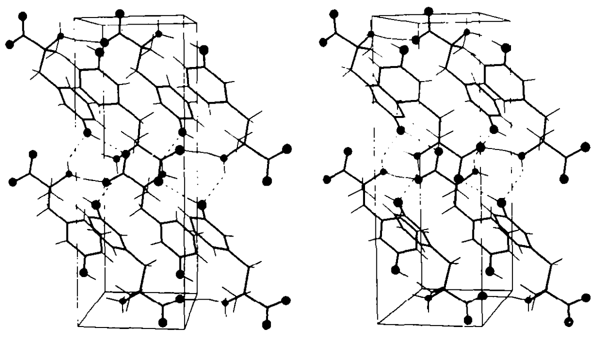

Fig. 2. Stereo packing diagram of MMT viewed down the *a* axis. Broken lines indicate H bonds.

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