Table 3. *Metal–chlorine bond lengths in indium*(III) *anions and related species*

Anion	*M*—Cl bond length (Å)	Reference
$InCl_4^-$,	2·33	Trotter, Einstein & Tuck (1969)
$InCl_5^{2-}$	2·42 (axial) 2·46 (basal)	Brown, Einstein & Tuck (1969)
	2·415 (axial) 2·495 (basal)	Joy *et al.* (1975)
$InCl_6^{3-}$	2·521	Present work
	2·523	Schlimper & Ziegler (1972)
$[InCl_3(H_2O)_3]$	2·447, 2·420, 2·399 (all *trans* to O)	Whitlow & Gabe (1975)
cis-$[InCl_4(H_2O)]^{2-}$	2·485 (*cis* to O) 2·425 (*trans* to O)	Ziegler *et al.* (1975)
$[InCl_5(H_2O)]^{2-}$	2·474 (*trans* to O) 2·463, 2·485, 2·486	Wignacourt, Mairesse & Barbier (1976)
$SnCl_6^{2-}$	2·43	Awasthi & Mehta (1969)
$CdCl_6^{4-}$	2·63	Bergerhoff & Schmitz-Dumart (1956)

values for In—Cl bonds *cis* and *trans* to In—OH_2. We conclude that all the In—Cl bond distances in Table 3 are satisfactorily accounted for by an ionic model of bonding in these complexes.

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N-Acetyl-L-tryptophan

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Abstract. $C_{13}H_{14}N_2O_3$, $M_r = 246·27$, orthorhombic, $P2_12_12_1$, $a = 7·470$ (1), $b = 25·912$ (4), $c = 6·247$ (1) Å, $Z = 4$, $D_m = 1·35$, $D_x = 1·353$ g cm^{-3}, $\mu = 8·17$ cm^{-1} (for Cu $K\alpha$). $R = 0·060$ for 626 non-zero reflexions. The molecular conformation shows good agreement with those of glycyl-L-tryptophan dihydrate and acetyl-L-tryptophan methyl ester.

Introduction. *N*-Acetyl-L-tryptophan was supplied by Drs Y. Shimonishi and S. Aimoto of the Institute for

Protein Research, Osaka University. The intensity data were collected on a Rigaku automatic four-circle diffractometer (AFC-III, at the Institute for Protein Research, Osaka University) with Ni-filtered Cu $K\alpha$ radiation. The crystal used for data collection had the dimensions 0·40 × 0·10 × 0·05 mm. 764 independent reflexions with $2\theta \le 100°$ were obtained by the ω-scan method. The scan width was 2·8° in 2ω. The intensity data were corrected for Lorentz and polarization effects.

The structure was solved by *MULTAN* (Germain, Main & Woolfson, 1970). The refinement was carried out by the block-diagonal least-squares method, with *HBLS* (Ashida, 1973). Anisotropic temperature factors for the heavy atoms and isotropic temperature factors for the H atoms were applied. In the refinement, the weights $\omega = a$ for $|F_o| = 0$, and $\omega = 1/(\sigma^2 + b \times |F_o| + c|F_o|^2)$ for $|F_o| \ne 0$ were assigned. The final refinement ($a = 0{\cdot}0892$, $b = 0{\cdot}0198$ and $c = 0{\cdot}0004$) gave an R of 0·105 for all reflexions (0·060 for 626 non-zero reflexions). The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Calculations were carried out on the FACOM 230-60 computer of the Computation Centre of Nagoya University. The final atomic parameters are listed in Tables 1 and 2.*

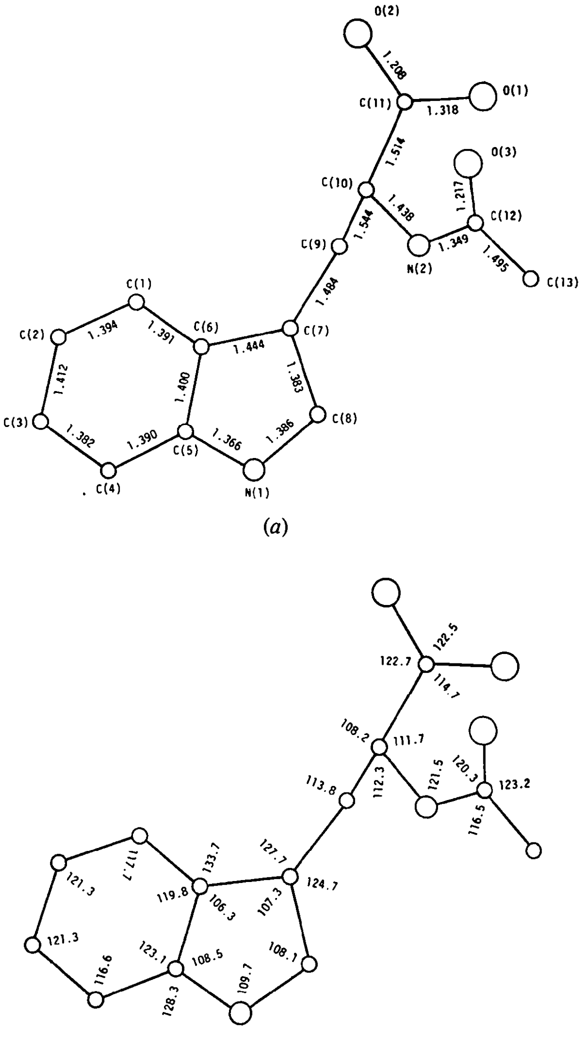
Discussion. The bond lengths and angles concerning the non-hydrogen atoms are shown in Fig. 1, together

Table 1. *Positional parameters* ($\times 10^4$), *with their standard deviations in parentheses*

	x	y	z
C(1)	−708 (10)	95 (3)	8655 (13)
C(2)	−979 (11)	−436 (3)	8532 (16)
C(3)	−480 (12)	−719 (3)	6696 (16)
C(4)	270 (11)	−479 (3)	4936 (13)
C(5)	538 (11)	51 (3)	5093 (13)
C(6)	135 (10)	335 (3)	6937 (12)
C(7)	653 (9)	861 (3)	6493 (13)
C(8)	1368 (11)	871 (3)	4451 (14)
N(1)	1266 (9)	377 (3)	3611 (11)
C(9)	623 (10)	1308 (3)	7980 (14)
C(10)	−1280 (11)	1494 (3)	8555 (13)
C(11)	−1115 (12)	1927 (3)	10171 (13)
O(1)	−1063 (9)	2393 (2)	9334 (8)
O(2)	−919 (9)	1849 (2)	12064 (8)
N(2)	−2279 (8)	1652 (2)	6698 (10)
C(12)	−3960 (11)	1837 (3)	6863 (13)
C(13)	−4778 (12)	2047 (3)	4859 (14)
O(3)	−4724 (7)	1838 (2)	8583 (9)

Table 2. *Positional parameters* ($\times 10^3$) *of hydrogen atoms with their standard deviations in parentheses*

	Bonded to	x	y	z
H(1)	C(1)	−72 (10)	21 (2)	1001 (11)
H(2)	C(2)	−143 (11)	−70 (3)	934 (13)
H(3)	C(3)	−75 (11)	−113 (3)	619 (14)
H(4)	C(4)	62 (13)	−64 (3)	328 (16)
H(5)	N(1)	161 (15)	30 (4)	242 (16)
H(6)	C(8)	173 (17)	124 (4)	383 (21)
H(7)	C(9)	122 (10)	170 (2)	752 (10)
H(8)		140 (10)	115 (2)	923 (11)
H(9)	C(10)	−183 (8)	113 (2)	901 (10)
H(10)	N(2)	−177 (10)	169 (3)	545 (12)
H(11)	O(1)	−49 (14)	279 (3)	1039 (17)
H(12)	C(13)	−580 (13)	186 (3)	464 (15)
H(13)		−555 (16)	248 (5)	528 (23)
H(14)		−409 (13)	201 (4)	361 (17)



(*a*)

(*b*)

Fig. 1. (*a*) Bond lengths (Å). (*b*) Bond angles (°).

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* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32494 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

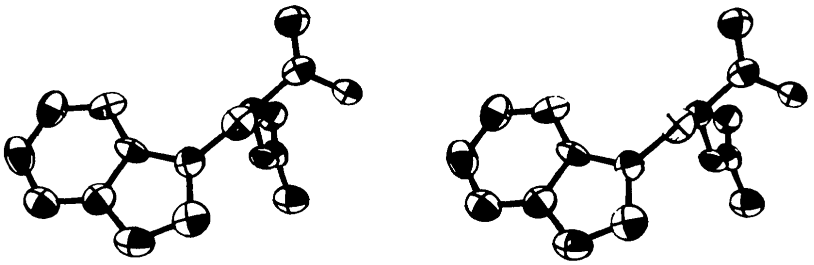

Fig. 2. A stereoscopic view showing vibration ellipsoids at 50% probability.

Table 3. *Best planes*

(*a*) Equations of the best planes

$$X = ax,\ Y = by,\ Z = cz$$

Plane I: Carboxyl group

$$0\cdot9936X - 0\cdot0482Y - 0\cdot1022Z + 1\cdot6920 = 0$$

Plane II: Peptide group

$$-0\cdot3386X - 0\cdot9211Y - 0\cdot1922Z + 4\cdot2263 = 0$$

Plane III: Indole ring

$$-0\cdot9087X + 0\cdot1939Y - 0\cdot3698Z + 1\cdot5337 = 0$$

(*b*) Displacements (×10³Å) of atoms from the planes. Atoms with asterisks are not included in the best-plane calculations.

(I)		(II)		(III)	
C(10)	9	C(10)	−43	C(1)	63
C(11)	−26	N(2)	56	C(2)	8
O(1)	8	C(12)	19	C(3)	−49
O(2)	9	C(13)	−34	C(4)	−30
N(2)*	−633	O(3)	3	C(5)	18
C(12)*	−1915	C(11)*	−1312	C(6)	8
C(13)*	−2421	O(1)*	−2338	C(7)	23
O(3)*	−2592	O(2)*	−1404	C(8)	14
C(7)*	1655	C(7)*	1226	N(1)	30
C(9)*	1482	C(9)*	−11	C(9)	−76
				C(10)*	1177

with the atom numbering system. The mean e.s.d.'s of the bond lengths and angles are 0·011 Å and 0·5° respectively. The equations of the best planes and the displacements of atoms from the planes are listed in Table 3. A stereoscopic view of the molecule drawn by *ORTEP* (Johnson, 1965) is shown in Fig. 2. The torsion angles are given in Table 4(*a*), together with those of glycyl-L-tryptophan dihydrate (Gly-L-Trp, Pasternak, 1956) and acetyl-L-tryptophan methyl ester (Ac-L-Trp-OMe, Cotrait & Barrans, 1974). The definition of the torsion angles given by the IUPAC–IUB Commission on Biochemical Nomenclature (1970) is adopted.

The conformations of the three molecules, except the χ^2 torsion angles, are surprisingly similar. In each of the three molecules, C^γ is *gauche* to N and *trans* to C′ with respect to the C^α—C^β bond. That is, χ^1 and the torsion angle of C′—C^α—C^β—C^γ are −59·6 and 176·7° in this molecule, −65·1 and 170·0° in Gly-L-Trp (Pasternak, 1956), and −64·7 and 172·4° in Ac-L-Trp-OMe (Cotrait & Barrans, 1974).

The structure of acetyl-L-tryptophan is described by the three planes of the carboxyl group, the peptide linkage and the indole ring. The dihedral angles

Table 4. *Torsion angles* (°) *and dihedral angles* (°)

(*a*) Torsion angles

	Reference	ω	φ	χ^1	$\chi^{2.1}$	$\chi^{2.2}$
Acetyl-L-tryptophan	1	172·9	−56·9	−59·6	116·5	−70·4
Glycyl-L-tryptophan dihydrate	2	−178·1	−72·9	−65·1	60·6	−122·3
Acetyl-L-tryptophan methyl ester	3	−176·5	−65·6	−64·7	88·0	−89·7

(*b*) Dihedral angles. The definition of the planes is given in Table 3.

	Reference	Between (I) & (II)	Between (I) & (III)	Between (II) & (III)
Acetyl-L-tryptophan	1	105·8	29·0	101·5
Glycyl-L-tryptophan dihydrate	2	92·4	29·8	106·6
Acetyl-L-tryptophan methyl ester	3	103·3	5·2	102·3

References: (1) This study. (2) Pasternak (1956). (3) Cotrait & Barrans (1974).

between the planes are given in Table 4(*b*). These dihedral angles are naturally in close agreement with those in Gly-L-Trp (Pasternak, 1956) and Ac-L-Trp-OMe (Cotrait & Barrans, 1974). On the other hand, the dihedral angles between the carboxyl plane and the indole ring of the tryptophans which have no peptide linkage at the amino N atom are usually much larger than in these three peptides: 70·6° in L-tryptophan hydrochloride (Takigawa, Ashida, Sasada & Kakudo, 1966), 53·2° in DL-tryptophan formate (Bye, Mostad & Rømming, 1973), 40·1° in 5-hydroxy-DL-tryptophan (Wakahara, Kido, Fujiwara & Tomita, 1973), and 61·5° in DL-tryptophan ethyl ester hydrochloride (Vijayalakshmi & Srinivasan, 1975).

The prominent feature of the crystal structure is the alternate stacking of the polar layer composed of the carboxyl and peptide groups and the non-polar layer of the indole ring along [010]. The N atom of the indole ring is not involved with the hydrogen bond. In the polar layer, two hydrogen bonds are observed: between O(1) and O(3) [$\frac{1}{2}+x, \frac{1}{2}-y, 2-z$], and between N(2) and O(2) [$x, y, -1+z$], the distances being 2·580 and 3·110 Å respectively.

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SHORT COMMUNICATION

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Acta Cryst. (1977). B**33**, 1653–1654

Single-crystal X-ray structure determination of ethylene at 85 K.

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Crystalline ethylene at 85 K is monoclinic, $a = 4{\cdot}626\ (1)$, $b = 6{\cdot}620\ (2)$, $c = 4{\cdot}067\ (2)$ Å, $\beta = 94{\cdot}39\ (2)°$, space group $P2_1/n$, $Z = 2$. Refinement of C and H parameters results in an $R = 0{\cdot}059$ for reflexions up to $\sin\theta/\lambda = 1{\cdot}07$ Å^{-1}.

Ethylene and other small hydrocarbons attract considerable attention because sophisticated theoretical calculations can relatively easily be done on these molecules in both the free and solid states. Up to now theoretical calculations on, for instance, solid ethylene are hampered by the lack of sufficiently reliable parameters (Elliott & Leroi, 1973). In the present paper we publish a single crystal X ray study of ethylene as part of an accurate study of the electron density distribution in single crystals of C_2H_2, C_2H_4 and C_2H_6.

Spherical ($\phi = 0{\cdot}58 \pm 0{\cdot}02$ mm) single crystals (mosaic spread $<0{\cdot}4°$) of C_2H_4 were grown *in situ* at 85 K on an Enraf–Nonius CAD-4 diffractometer. The reflexion symmetry $I(hkl) = I(h\bar{k}l)$ and the systematic extinctions $h0l$ ($h + l = 2n + 1$) and $0k0$ ($k = 2n + 1$) indicated the space group $P2_1/n$, in agreement with Elliott & Leroi (1973), Ligthart (1975) and Brecher & Halford (1961). Cell dimensions were determined from θ, φ, ω and κ reflexion angles, measured on the diffractometer.

The observed values of $a = 4{\cdot}626\ (1)$, $b = 6{\cdot}620\ (2)$, $c = 4{\cdot}067\ (2)$ Å and $\beta = 94{\cdot}39\ (2)°$ are consistent with those given by Ligthart (1975). Intensities were collected by the θ–2θ scan technique with graphite-monochromatized Mo $K\alpha$