expected, this is found to be the case. For the monodentate group (HTFA), the small but significant barrier to rotation predicted by the *GAUSSIAN*90 calculation would be superimposed on the intermolecular effects to give a distribution of angles favouring the minimum energy conformation. The database analysis is in agreement with this, indicating a bias towards the eclipse of the C—F bond by C=O rather than C—O—.

A comparison of the mean distances observed with those calculated indicates that, in general, the latter are always greater. Corrections for libration of the group as a rigid body and for internal rotation would increase the observed values, particularly the C—F distances. An unexplained feature is the shortening of the C—O— distance in monodentate structures compared with the calculated value. It will be of interest to investigate this feature in other carboxylic acid structures.

We acknowledge the use of the Cambridge Structural Database (Allen *et al.*, 1991) and of the EPSRC's Chemical Database Service at Daresbury.

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# X-ray Studies on Crystalline Complexes Involving Amino Acids and Peptides. XXVIII. Recurrence of Characteristic Aggregation and Interaction Patterns in the Crystal Structures of DL- and L-Lysine Formate

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## Abstract

The crystal structures of L-lysine formate [$P2_1$, $a = 5.431$ (1), $b = 7.546$ (1), $c = 12.095$ (2) Å, $\beta = 93.42$ (1)°, $Z = 2$] and DL-lysine formate [$P2_1/c$, $a = 10.205$ (2), $b = 11.152$ (2), $c = 8.491$ (1) Å, $\beta = 97.51$ (1)°, $Z = 4$] have been determined and refined to $R = 0.039$ and 0.054 for 1060 and 1689 observed reflections, respectively. Both the structures consist of alternating layers of unlike molecules. The aggregation pattern in the lysine layer in the L-lysine complex, with a straight and a zigzag head-to-tail sequence interconnecting the molecules, is almost the same as that observed in L-lysine acetate, L-lysine L-aspartate and L-lysine D-aspartate. In the DL-lysine complex, hydrogen-bonded dimers of lysine are interconnected by head-to-tail sequences, as in DL-lysine hydrochloride. The structures thus demonstrate the relative invariance of certain aggregation and interaction patterns involving lysine. The relative invariance also extends to interactions between the side-chain amino group and the formate ions.

## Introduction

We have been investigating the crystalline complexes involving amino acids and peptides in a long-range programme aimed at elucidating the atomic details of biologically and evolutionary important non-covalent

interactions (Vijayan, 1988; Prasad & Vijayan, 1993; Suresh, Prasad & Vijayan, 1994). These investigations have brought to light several specific interactions and characteristic interaction and aggregation patterns (Vijayan, 1988; Suresh & Vijayan, 1983*a*; Suresh and Vijayan, 1985). In addition to their intrinsic interest in relation to molecular association in general, they appear to have implications on chemical evolution (Vijayan, 1980, 1988). The current phase of the programme on the complexes is concerned with amino acids and peptides with other small molecules which are believed to have existed in the prebiotic milieu. The complexes have provided interesting information relevant to the self-assembly processes that might have given rise to primitive multimolecular systems (Prasad & Vijayan, 1993; Suresh, Prasad & Vijayan, 1994). Formic acid is the most abundant carboxylic acid found in experiments designed to simulate prebiotic organic synthesis (Miller & Urey, 1959; Kvenvolden, Lawless & Ponnamperuma, 1971; Miller & Orgel, 1974) and here we report the crystal structures of the complexes of formic acid with DL- and L-lysine, which demonstrate the relative invariance of amino acid aggregation with respect to the size and nature of the other molecules or ions in the system.

## Methods

Crystals of both complexes were grown by the slow diffusion of acetonitrile into aqueous solutions of the components. The cell parameters were refined on a computer-controlled CAD-4 diffractometer, which was also used to collect the intensity data. The crystal data, experimental details and refinement parameters are given in Table 1.

The structures were solved using the direct-methods program *SHELXS*86 (Sheldrick, 1985) and refined by the full-matrix least-squares method employing a minimization function based on $F^2$, using the program *SHELXL*93 (Sheldrick, 1993). The H atoms were located from difference-Fourier maps using stereochemical considerations. Non-H atoms were refined ansiotropically and H atoms isotropically. The positional parameters and equivalent isotropic thermal parameters in the two structures are given in Tables 2 and 3.*

### *Twinning*

The crystals of DL-lysine formate are twinned as illustrated in Fig. 1. The disposition of the major and minor twin components is such that their reflections are separable, except when $l = 3n$ ($n$ = integer). Only the reflections corresponding to the major component were used in structure analysis and refinement. The contribution from the minor component to reflections with $l = 3n$ was taken into account during refinement using the provision for doing so in the structure refinement package *SHELXL*93 (Sheldrick, 1993). The ratio between the major and minor components refined to 93:7. Despite the presence of twinning, the structure refined reasonably well, except that the final difference-Fourier map was noisy. The peaks in the map could not, however, be explained in a chemically sensible manner.

Table 1. *Crystal data, experimental details and refinement parameters for* L-*lysine formate and* DL-*lysine formate (e.s.d.'s in parentheses)*

| | L-Lysine formate | DL-Lysine formate |
|---|---|---|
| Chemical formula | $C_6H_{15}N_2O_2^+.CHO_2^-$ | $C_6H_{15}N_2O_2^+.CHO_2^-$ |
| Formula weight | 192.22 | 192.22 |
| Crystal system | Monoclinic | Monoclinic |
| Space group | $P2_1$ | $P2_1/c$ |
| Unit-cell dimensions | | |
| $a$ (Å) | 5.431 (1) | 10.205 (2) |
| $b$ (Å) | 7.546 (1) | 11.152 (2) |
| $c$ (Å) | 12.095 (2) | 8.481 (1) |
| $\beta$ (°) | 93.42 (1) | 97.51 (1) |
| Volume (Å$^3$) | 494.8 (1) | 956.9 (2) |
| $Z$ | 2 | 4 |
| $D_x$ (Mg m$^{-3}$) | 1.290 | 1.334 |
| $D_m$ (Mg m$^{-3}$) | 1.29 (2) | 1.35 (2) |
| Crystal size (mm) | 0.50 × 0.19 × 0.07 | 0.35 × 0.30 × 0.06 |
| Wavelength (Å) | 1.5418 | 1.5418 |
| Absorption coefficients (mm$^{-1}$) | 0.890 | 0.920 |
| Absorption correction | None | None |
| Extinction correction | Empirical | None |
| Extinction coefficient | 0.031 (6) | |
| Number of reflections for lattice parameters | 25 | 25 |
| $\theta$ range for lattice parameters (°) | 16–37 | 4–37 |
| Maximum Bragg angle ($\theta$, °) | 75 | 75 |
| $h$ range | 0–6 | 0–12 |
| $k$ range | 0–9 | 0–13 |
| $l$ range | −15–15 | −10–10 |
| Reflections measured | 1210 | 2080 |
| Unique reflections | 1094 | 1970 |
| Reflections observed [$F > 4\sigma(F)$] | 1060 | 1689 |
| $R_{int}$ | 0.052 | 0.020 |
| Parameters refined | 183 | 183 |
| Weighting function | $1/[\sigma_{F_o}^2 + (0.0844P)^2 + 0.0484P]$ where $P = (F_o^2 + 2F_c^2)/3$ | $1/[\sigma_{F_o}^2 + (0.0983P)^2 + 0.5895P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Goodness-of-fit on $F^2$ | 1.046 | 1.181 |
| $R$ [$F > 4\sigma(F)$] | 0.0388 | 0.0539 |
| $wR_2$ (all data) | 0.1069 | 0.1935 |
| $(\Delta/\sigma)_{max}$ | 0.035 | 0.021 |
| $(\Delta\rho)_{max}$ (e Å$^{-3}$) | 0.348 | 1.045 |
| $(\Delta\rho)_{min}$ (e Å$^{-3}$) | −0.183 | −0.937 |

## Results and discussion

### *Molecular dimensions*

The lysine molecule in both the structures is zwitterionic with positively charged $\alpha$- and side-chain amino groups, and a negatively charged $\alpha$-carboxylate group. The positive charge is compensated by the negatively charged formate ion. The torsion angles that

* Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AS0672). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^4$) *for* L-lysine formate

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| O(1) | 12378 (3) | −69 (3) | 6289 (1) | 387 (5) |
| O(2) | 12465 (3) | 1955 (2) | 4960 (1) | 373 (5) |
| N(1) | 7460 (3) | −18 (2) | 6294 (2) | 258 (5) |
| C(1) | 11416 (3) | 1103 (3) | 5670 (2) | 269 (5) |
| C(2) | 8701 (4) | 1569 (3) | 5861 (2) | 254 (5) |
| C(3) | 8679 (4) | 3112 (3) | 6681 (2) | 301 (5) |
| C(4) | 6120 (4) | 3823 (3) | 6892 (2) | 333 (6) |
| C(5) | 6241 (4) | 5376 (3) | 7702 (2) | 364 (6) |
| C(6) | 3790 (5) | 6329 (3) | 7703 (2) | 371 (7) |
| N(7) | 3783 (4) | 7764 (3) | 8543 (2) | 369 (6) |
| O(11) | 953 (4) | 4295 (3) | 11417 (2) | 490 (6) |
| O(12) | 3444 (4) | 5962 (4) | 10505 (2) | 665 (8) |
| C(11) | 1405 (5) | 5389 (5) | 10687 (2) | 485 (9) |

Table 3. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^4$) *for* DL-*lysine formate*

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| O(1) | 5478 (2) | 3688 (2) | 4241 (2) | 352 (6) |
| O(2) | 4603 (2) | 2338 (2) | 2493 (2) | 395 (6) |
| N(1) | 3129 (2) | 4106 (2) | 5300 (2) | 276 (6) |
| C(1) | 4521 (2) | 3186 (2) | 3463 (3) | 264 (6) |
| C(2) | 3134 (2) | 3641 (2) | 3647 (3) | 257 (7) |
| C(3) | 2703 (3) | 4651 (2) | 2470 (3) | 305 (7) |
| C(4) | 2389 (3) | 4232 (2) | 750 (3) | 361 (8) |
| C(5) | 1994 (3) | 5265 (3) | −403 (3) | 366 (8) |
| C(6) | 3191 (3) | 5991 (3) | −707 (3) | 344 (9) |
| N(7) | 2827 (2) | 7084 (2) | −1663 (2) | 303 (7) |
| O(11) | −1437 (2) | 3389 (2) | 4614 (2) | 427 (6) |
| O(12) | 579 (2) | 3629 (2) | 5928 (3) | 518 (8) |
| C(11) | −216 (3) | 3535 (3) | 4723 (4) | 393 (9) |

define the conformation of the molecules (IUPAC-IUB Commission on Biochemical Nomenclature, 1970) are given in Table 4. The side chain is in the fully extended conformation in L-lysine formate. In fact, the lysyl side chain has a proclivity to occur in the all *trans* conformation; 14 of the 19 independent lysine molecules observed in crystal structures so far have $\chi^2$-, $\chi^3$- and $\chi^4$-values close to 180° (Prasad & Vijayan, 1991). The side chain is *trans* to the $\alpha$-carboxylate group

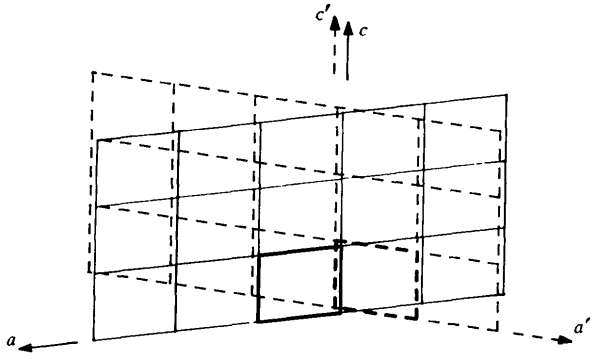


Fig. 1. Superposition of the direct lattices of the two twin components in the crystals of DL-lysine formate. The lattice of one twin component is drawn in continuous lines, and the other in dashed lines.

Table 4. *Torsion angles of lysine in* L- *and* DL-*lysine formate* (°)

| | $\psi'$ | $\chi^1$ | $\chi^2$ | $\chi^3$ | $\chi^4$ |
|---|---|---|---|---|---|
| L-Lysine formate | −29.3 (2) | −64.5 (2) | −179.1 (2) | 167.0 (2) | 175.7 (2) |
| DL-Lysine formate | −31.4 (3) | −167.9 (2) | −178.6 (2) | 75.7 (3) | −173.1 (2) |

($\chi^1 \sim -60°$), in L-lysine formate, as in eight of these 14 molecules. The conformation of the side chain in DL-lysine formate is folded as in DL-lysine hydrochloride (Bhaduri & Saha, 1979). The orientation of the side chain with respect to the main chain atoms is also similar in the two structures with $C^\gamma$ *trans* to the $\alpha$-amino group ($\chi^1 \sim 180°$).

### *Molecular aggregation*

The crystal structures of the two complexes are illustrated in Figs. 2 and 3, whilst Table 5 lists the hydrogen-bond parameters.

The amino acid molecules in L-lysine formate (Fig. 2) aggregate into layers perpendicular to the *c*-axis. In each layer (Fig. 4), the molecules are held together by two sets of head-to-tail sequences (Suresh & Vijayan, 1983*a*) in which the $\alpha$-amino and $\alpha$-carboxylate groups are brought into periodic hydrogen-bonded proximity in a polypeptide arrangement. One such group, termed *S*1 (Suresh & Vijayan, 1983*a*), involves a N(1)—H···O(1) hydrogen bond between two molecules related by an *a* translation and its symmetry equivalents. The other, termed *Z*2, is made up of a N(1)—H···O(2) hydrogen bond between molecules related by a $2_1$ screw parallel to *b* and its symmetry equivalents. Thus, according to the nomenclature we used to describe amino acid aggregation (Suresh & Vijyan, 1983*a*), the planar aggregation of lysine molecules in the structure (Fig. 4) is of the *S*1*Z*2 type. Indeed, aggregation involving the coexistence of a straight (*S*) and a zigzag (*Z*) sequence is a feature observed in the crystal structures of most hydrophilic amino acids (Vijayan, 1988; Soman & Vijayan, 1989). In L-lysine formate, the lysine layers are interconnected by interactions involving formate ions.

It turns out that the formation of *S*1*Z*2 layers involving L-lysine molecules occurs in the crystal structures of L-lysine acetate (Suresh & Vijayan, 1983*b*), L-lysine L-aspartate (Bhat & Vijayan, 1974) and L-lysine D-aspartate monohydrate (Soman, Suresh & Vijayan, 1988) also. For comparison, the space group and the unit-cell parameters of these crystals are given in Table 6. In all the crystals, the layers are in the *ab*-plane. The *S*1 sequences run along *a* and the dimension *ca* 5.5 Å represents a link in this sequence. The *Z*2 sequences centred around $2_1$ screw axes are parallel to *b* and have a periodicity ranging from 7.15 to 7.85 Å. In all four complexes, the unlike molecules aggregate into alternating layers stacked along *c*. Thus, the *c*-translation is determined by the thickness of both the L-lysine layer,

which is almost the same in all the structures, and the layer containing the anions. The formate is the smallest of the relevant ions and thus the *c*-dimension is the least in L-lysine formate. The larger size of the acetate ion is reflected in the larger *c*-dimension in L-lysine acetate. The aspartate ion is still larger and hence the *c*-translation in L-lysine L-aspartate has a still larger value. L-Lysine D-aspartate crystallizes in the space group $P2_12_12_1$ with $Z = 4$, unlike the other three complexes which crystallize in the space group $P2_1$ with $Z = 2$. Furthermore, it additionally contains water of crystallization. Consequently, although the L-lysine layers are of the *S*1Z2 type, as in the other three complexes, the *c*-dimension in L-lysine D-aspartate monohydrate is more than twice that in L-lysine L-aspartate, the effect being further accentuated by a compensating reduction in the *b*-dimension.

In DL-lysine formate also, the molecules aggregate into alternating layers (Fig. 3). In the lysine layer, illustrated in Fig. 5, the molecules form dimers across inversion centres, each dimer stabilized by a N(1)—H···O(1) hydrogen bond and its centrosymmetric equivalent.

Table 5. *Hydrogen-bond parameters in* L- *and* DL-*lysine formate*

| *A*—H···*B* | *A*···*B* (Å) | *A*—H···*B* (°) |
|---|---|---|
| L-Lysine formate | | |
| N(1)—H(1)N(1)···O(1$^{i}$) | 2.760 (2) | 174 (3) |
| N(1)—H(2)N(1)···O(11$^{ii}$) | 2.897 (3) | 173 (3) |
| N(1)—H(3)N(1)···O(2$^{iii}$) | 2.744 (3) | 154 (3) |
| N(7)—H(1)N(7)···O(11$^{iv}$) | 2.823 (3) | 172 (4) |
| N(7)—H(2)N(7)···O(12$^{v}$) | 2.751 (3) | 165 (4) |
| N(7)—H(3)N(7)···O(11$^{vi}$) | 3.081 (3) | 158 (4) |
| DL-Lysine formate | | |
| N(1)—H(1)N(1)···O(12$^{v}$) | 2.775 (3) | 156 (3) |
| N(1)—H(2)N(1)···O(2$^{vii}$) | 2.754 (3) | 174 (3) |
| N(1)—H(3)N(1)···O(1$^{viii}$) | 2.843 (3) | 179 (3) |
| N(7)—H(1)N(7)···O(11$^{ix}$) | 2.792 (3) | 164 (3) |
| N(7)—H(2)N(7)···O(11$^{x}$) | 2.762 (3) | 177 (3) |
| N(7)—H(3)N(7)···O(2$^{xi}$) | 2.876 (3) | 158 (3) |

Symmetry codes: (i) $+x-1, +y, +z$; (ii) $-x+1, +y-\frac{1}{2}, -z+2$; (iii) $-x+2, +y-\frac{1}{2}, -z+1$; (iv) $-x, +y+\frac{1}{2}, -z+2$; (v) $x, y, z$; (vi) $-x+1, +y+\frac{1}{2}, -z+2$; (vii) $+x, -y+\frac{1}{2}, +z+\frac{1}{2}$; (viii) $-x+1, -y+1, -z+1$; (ix) $-x, +y+\frac{1}{2}, -z+\frac{1}{2}$; (x) $-x, -y+1, -z$; (xi) $-x+1, -y+1, -z$.

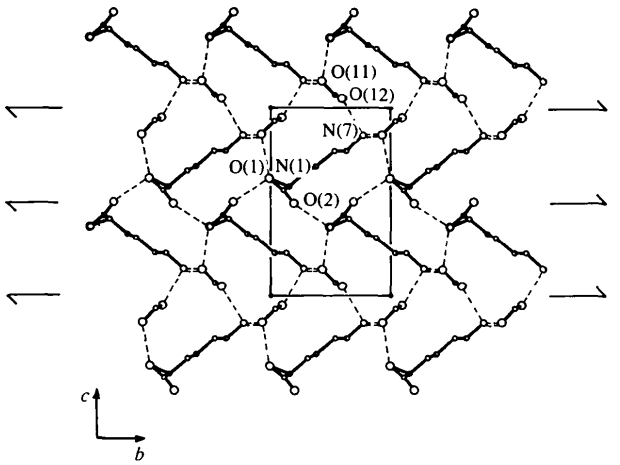


Fig. 2. The crystal structure of L-lysine formate. O, N and C atoms are represented by spheres of decreasing size, and also in subsequent figures [drawn using *PLUTO* (Motherwell & Clegg, 1978)].

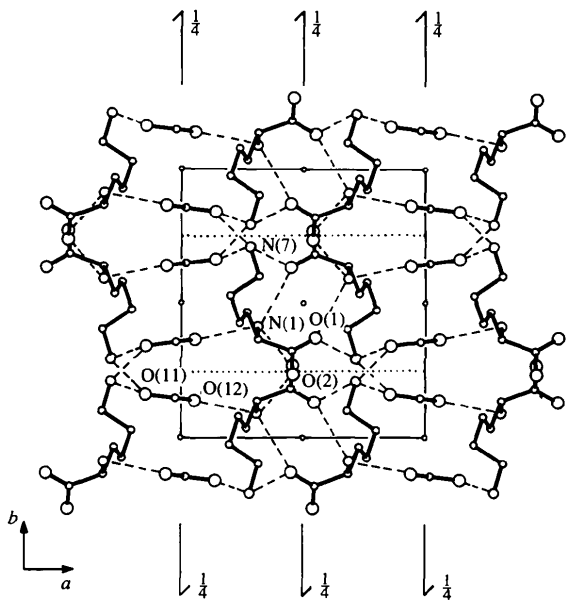


Fig. 3. The crystal structure of DL-lysine formate [drawn using *PLUTO* (Motherwell & Clegg, 1978)].

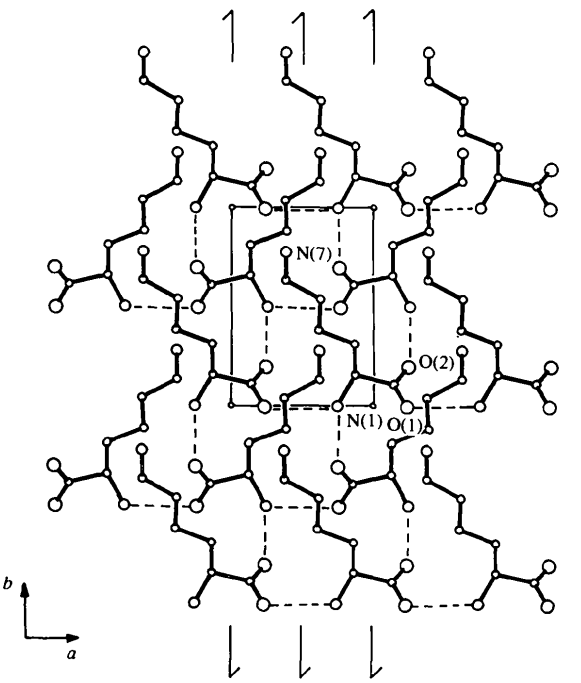


Fig. 4. The arrangement of molecules in the lysine layer of L-lysine formate [drawn using *PLUTO* (Motherwell & Clegg, 1978)].

Table 6. *Space groups and cell parameters of some crystalline complexes containing* L-*lysine*

| Complex | Space group | *a* (Å) | *b* (Å) | *c* (Å) | *β* (°) |
|---|---|---|---|---|---|
| L-Lysine acetate | $P2_1$ | 5.411 (1) | 7.562 (1) | 12.635 (2) | 91.7 (1) |
| L-Lysine L-aspartate | $P2_1$ | 5.555 (6) | 7.867 (6) | 15.376 (15) | 99.1 (1) |
| L-Lysine D-aspartate monohydrate | $P2_12_12_1$ | 5.458 (1) | 7.152 (2) | 36.022 (5) | — |

These hydrogen-bonded dimers are interconnected through DL2 head-to-tail sequences (Suresh & Vijayan, 1983*a*) formed by a N(1)—H···O(2) hydrogen bond between two *c*-glide-related molecules and their symmetry equivalents. N(7)—H···O(2) side-chain–main-chain hydrogen bonds lend further stability to the lysine layer. The lysine layers are again interconnected through formate ions.

Interestingly, the crystal structure of DL-lysine formate is very similar to that of DL-lysine hydrochloride (Bhaduri & Saha, 1979), except that the formate ion is replaced by the chloride ion. Both the structures have the same space group with comparable unit-cell dimensions. Molecular aggregation in the two crystals is essentially the same in nature. Indeed, dimerization across inversion centres stabilized by hydrogen bonds involving main chain atoms is a feature observed in many crystal structures containing DL-amino acids. Such dimerization also occurs in the complexes of DL-lysine with acetic acid (Soman, Rao, Radhakrishnan & Vijayan, 1989) and succinic acid (Prasad & Vijayan, 1991), except that N(1)—H···O(2) hydrogen bonds are involved in the dimerization in these two complexes rather than the N(1)—H···O(1) hydrogen bonds in DL-lysine formate and DL-lysine hydrochloride. However, unlike in the corresponding L-lysine complexes, there is no striking similarity between the structures of DL-lysine formate and DL-lysine acetate. The succinic acid complex of DL-lysine has elements of similarity with DL-lysine acetate and DL-lysine formate, but the overall aggregation patterns in the three complexes are not of the same type.

### *Lysine–formate interactions*

From the point of view of molecular aggregation, the formate ions are involved in interconnecting lysine layers in both structues. As in the case of the corresponding acetates, the lysine molecules in the structures interact with the formate ions primarily through the side-chain amino groups. These interactions essentially assume the characteristic pattern (Vijayan, 1988) involving a linear array of alternating amino and carboxylate groups, a situation also encountered in many other crystal structures containing lysine. In L-lysine formate, there are two such arrays along *b*, each centred around a $2_1$ screw axis, together giving rise to a third array parallel to *a* involving amino and carboxylate groups related by cell translations, completing a two-dimensional network, as illustrated in Fig. 6. The structure of DL-lysine formate (Fig. 3) contains one linear array of alternating side-chain amino groups and formate ions related by a glide plane.

Studies of complexes of amino acids and peptides (Vijayan, 1988; Soman & Vijayan, 1989) suggest that these molecules follow a few, often predictable, basic patterns of aggregation and interaction which are substantially preserved with respect to variations in the size and nature of other molecules present in the system. The crystal structures of the two complexes further demonstrate the relative invariance of some of these patterns.

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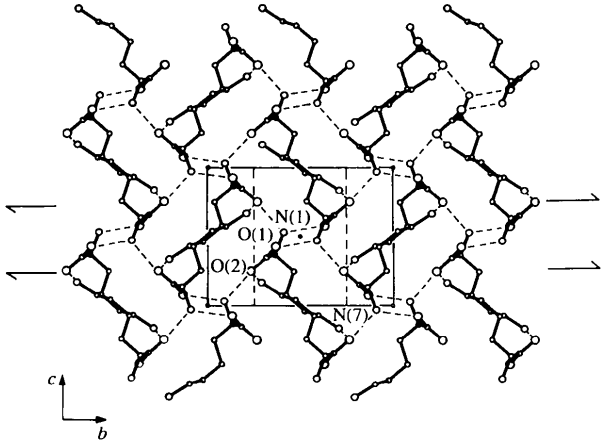


Fig. 5. The arrangement of molecules in the lysine layer of DL-lysine formate [drawn using *PLUTO* (Motherwell & Clegg, 1978)].

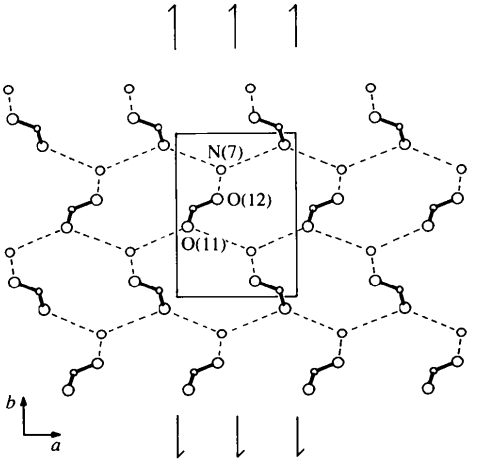


Fig. 6. Characteristic interaction patterns in L-lysine formate forming a layer in the *ab*-plane [drawn using *PLUTO* (Motherwell & Clegg, 1978)].

Industrial Research, India. The computations were performed in the Supercomputer Education and Research Centre at the Institute.

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# Structure of 9-Deoxo-9a-*N*-[*N'*-(4-pyridyl)-carbamoyl]-9a-aza-9a-homoerythromycin A and Conformational Analysis of Analogous 9a-Aza 15-Membered Azalides in the Solid State

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## Abstract

$C_{43}H_{74}N_4O_{13}.C_3H_6O$, $M_r$ = 913, triclinic, $P1$, $a$ = 10.3796 (5), $b$ = 14.5809 (5), $c$ = 17.1521 (9) Å, $\alpha$ = 105.225 (3), $\beta$ = 96.140 (5), $\gamma$ = 90.248 (3)°, $V$ = 2489.0 (2) Å$^3$, $Z$ = 2 (two independent molecules in the asymmetric unit), $D_x$ = 1.218 g cm$^{-3}$, $\lambda$(Cu $K\alpha$) = 1.54184 Å, $T$ = 106 (3) K, $F(000)$ = 992, $\mu$(Cu $K\alpha$) = 7.0 cm$^{-1}$, $R$ = 0.057 for 8724 observed unique reflections with $I > 2\sigma(I)$. Conformational analysis is based on X-ray structure determinations of 9-deoxo-9a-*N*-[*N'*-(4-pyridyl)-carbamoyl]-9a-aza-9a-homoerythromycin A (1) and its *N*-isopropyl-carbamoyl congener (2) and data for 9a-aza 15-membered azalides retrieved from the Cambridge Structural Database (Version 5.07). The analysis reveals that the aglycone ring conformation has been influenced by the presence or absence of glyco conjugation at C3 and C5 sites in azalide derivatives. However, more drastic influence is related to the appearance of intramolecular hydrogen bonds. Compounds with 9a N atoms in $sp^3$ hybridization exhibit N—H···O contacts which are absent in compounds with 9a N atoms in $sp^2$ hybridization; they reveal O—H···O intramolecular hydrogen bonds. The 15-membered azalides studied are in 'folded-out' conformation in the solid state. The $\alpha$-L-cladinose sugar moiety is in $^1C_4$ conformation, while the $\beta$-D-desosamine adopts a $^4C_1$ conformation. The absolute configurations at the aglycone chiral centres are as follows: *C2R*, *C3S*, *C4S*, *C5R*, *C6R*, *C8R*, *C10R*, *C11R*, *C12S* and *C13R*.


## Introduction

9-Deoxo-9a-*N*-[*N'*-(4-pyridyl)-carbamoyl]-9a-aza-9a-homoerythromycin A (1) is a member of the novel series of 9-deoxo-9a-(*N*-substituted-carbamoyl)-9a-aza-9a-homoerythromycin A compounds (Kujundžić,

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