3374 reflections
253 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.4855P]$
where $P = (F_o^2 + 2F_c^2)/3$

Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 5. *Selected geometric parameters (Å, °) for (III)*

S2—C21	1.807 (3)	N1—C16	1.529 (3)
S1—C11	1.808 (3)	N2—C22	1.526 (3)
N1—C12	1.515 (3)	N2—C23	1.525 (4)
N1—C13	1.524 (3)	N2—C26	1.530 (3)
C21—S2—H2*S*	96.2 (16)	C16—N1—H1	106.2
C11—S1—H1*S*	96.3 (16)	C22—N2—C23	112.2 (2)
C12—N1—C13	112.4 (2)	C22—N2—C26	111.0 (2)
C12—N1—C16	112.0 (2)	C23—N2—C26	115.1 (2)
C13—N1—C16	113.3 (2)	C22—N2—H2	105.9
C12—N1—H1	106.2	C23—N2—H2	105.9
C13—N1—H1	106.2	C26—N2—H2	105.9
H13—C13—N1—H1	−174.9	H23—C23—N2—H2	−61.1
H16—C16—N1—H1	−61.0	H26—C26—N2—H2	−172.5
N1—C12—C11—S1	177.0 (2)	N2—C22—C21—S2	175.7 (2)

Table 6. *Hydrogen-bonding geometry (Å, °) for (III)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1$^{\rm i}$	0.91	2.26	3.155 (2)	166.3
C11—H11*A*···S2$^{\rm ii}$	0.97	2.89	3.670 (3)	138.4
C13—H13···Cl2$^{\rm iii}$	0.98	2.84	3.707 (3)	148.0
C24—H24*B*···Cl2	0.96	2.93	3.703 (4)	137.8
C26—H26···Cl1$^{\rm iv}$	0.98	2.95	3.873 (3)	157.8
S1—H1*S*···Cl1	1.23 (2)	2.59 (2)	3.799 (1)	169 (2)
N2—H2···Cl2	0.91	2.24	3.128 (2)	166.4
S2—H2*S*···Cl2$^{\rm v}$	1.24 (2)	2.47 (2)	3.694 (1)	169 (2)

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y-1, 1+z$; (iii) $\frac{3}{2}-x, y, \frac{1}{2}+z$; (iv) $1-x, 1-y, z-\frac{1}{2}$; (v) $x, 1+y, z$.

A full sphere [(I) and (II)] or hemisphere [(III)] of reciprocal space was scanned by 0.3° steps in ω with a crystal-to-detector distance of 6.22 cm. The non-H atoms were refined anisotropically. H(—S) atoms were refined isotropically with a restrained S—H distance, whereas other H atoms were treated isotropically using an appropriate riding model.

For all compounds, data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT* and *SADABS* (Sheldrick, 1996); program(s) used to solve structures: *SHELXS*97 (Sheldrick, 1997*b*); program(s) used to refine structures: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*c*).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1104). Services for accessing these data are described at the back of the journal.

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(1*S*,2*R*)-1-Amino-2-methoxycyclohexane-1-carboxamide hydrochloride 0.25-hydrate

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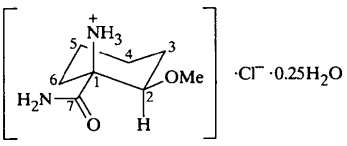
Abstract

The title compound, (1-carboxamido-2-methoxycyclohexyl)ammonium chloride 0.25-hydrate, $C_8H_{17}N_2O_2^+\cdot Cl^-\cdot 0.25H_2O$, (I), was obtained in the course of our research efforts towards 2,4-propano analogues of the naturally occurring α-amino acid $\rm L_s$-threonine. In order to elucidate the absolute stereochemistry of (I), the absolute configuration was determined by exploiting anomalous dispersion effects. The crystal structure contains four independent molecules within the asymmetric unit, which are linked by a network of hydrogen bonds and include the Cl^- ions. The absolute configuration of all four molecules is the same; however, differences in the conformation of some groups are present.

Comment

It has been shown that the asymmetric Strecker synthesis is a valuable tool for the preparation of 2-substituted carbocyclic α-amino acids (Volk & Frahm, 1996). Although interesting pharmacological properties of some 2-hydroxylated aminocyclohexanecarboxylic acids have been described recently (Horikawa *et al.*, 1998), the results were not conclusive in terms of structure–activity relationships. We therefore planned to prepare a complete set of stereomeric 1-amino-2-hydroxycyclohexanecarboxylic acids. Starting from (*R*)- and (*S*)-1-phenylethylamine, 2-methoxycyclohexanone and trimethylsilylcyanide, all four possible stereoisomers can be obtained *via* asymmetric Strecker synthesis (Pai Fondekar *et al.*, 1999). The relative stereochemistry of the title compound, (I) (Fig. 1), was deduced on the basis of NMR experiments. Thus, the heteronuclear coupling constant of 1.6 Hz between the carboxamide C7 atom and the proton H21 clearly indicates the *cis* configuration according to the Karplus curve (Karplus, 1963), with a C7—C1—C2—H21 torsion angle of ~ 60°. In contrast, the respective *trans*-configured isomer showed a *J* value of 6.3 Hz. Since (I) was prepared using (*S*)-1-phenylethylamine as the chiral auxiliary, a (1*S*,2*R*) configuration was predicted. This absolute configuration has now been confirmed by X-ray analysis.



(I)

The *cis*-substitution pattern at the C1 and C2 positions of the cyclohexane ring is demonstrated by the torsion angles C7—C1—C2—H21 = 54.7 (10), N1—C1—C2—H21 = 171.8 (10), C7—C1—C2—O1 = −68.3 (1) and N1—C1—C2—O1 = 48.7 (1)°. The cyclohexane ring shows the expected chair conformation, with the carboxamide at C1 and the methoxy at C2 both in equatorial positions, and the ammonium group at C1 in an axial position. In solution, compound (I) adopts the alternative chair conformation, with the opposite equatorial and axial orientations for the substituents at C1 and C2 (Pai Fondekar *et al.*, 1999).

The torsion angles for the other three molecules in the asymmetric unit show deviations of up to ~ 6° from the values for the first molecule (Table 1). The labelling is as follows: first molecule, C1–C7, N1, N2, O1, O2; add 10, 20 and 30 for the second, third and fourth molecules, respectively. H atoms bonded to C atoms are labelled with ten times the number of the C atom plus 1 or 2; for H atoms bound to N atoms, *A*, *B* and *C* are appended instead of 1 or 2.

The conformation of the cyclohexane rings is the same for all four molecules. All bond distances of the

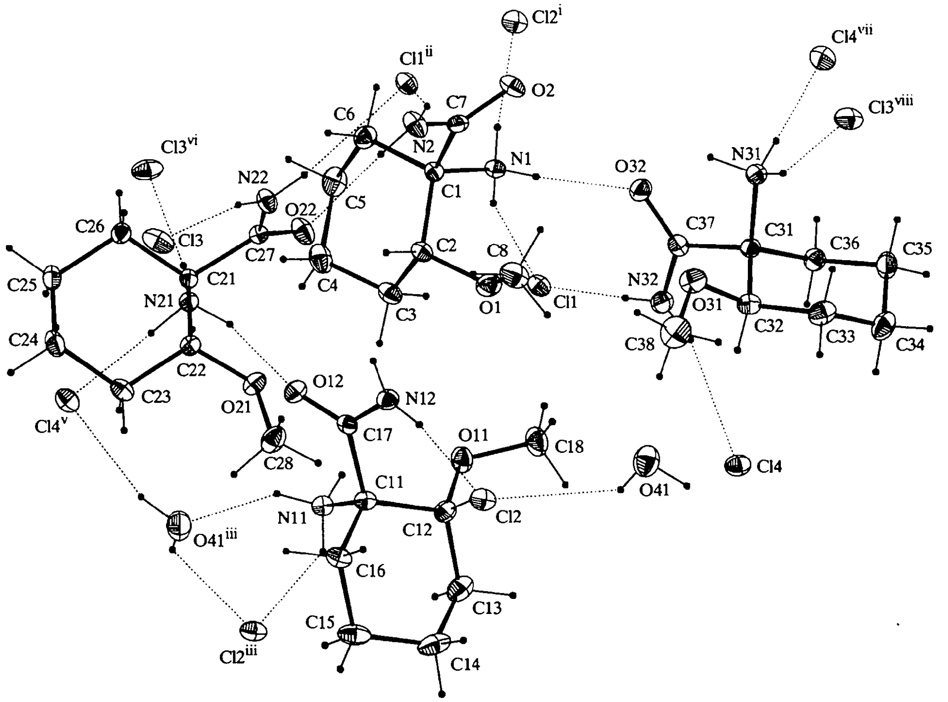


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids for non-H atoms and the atom-numbering scheme. H atoms are drawn as filled circles. All four independent molecules are shown. For some Cl^- ions and the water molecule, symmetry-equivalent positions are also shown, in order to illustrate the hydrogen bonds; symmetry codes are as in Table 2. The N11···O2^{iv} and O41···Cl4^{ix} hydrogen bonds are not shown.

corresponding atoms of the different molecules agree within experimental errors (Table 1). However, the bond angles, especially of O1 (O11, O21, O31) show variations of up to ~5° between different molecules. This is mainly due to the disparate C8—O1—C2—C1 torsion angle of 82.1 (2)° for the first molecule, compared with the corresponding values of 156–172° for the other three molecules. This significant difference in conformation (Fig. 1) is associated with other smaller changes in torsion and bond angles (Table 1).

All molecules are linked in three dimensions by a number of hydrogen bonds which include all the Cl^- ions, as well as an additional water molecule (Table 2 and Fig. 1). Only two of all of the possible N—H(···) donors (at N12 and N31) form no hydrogen bonds.

Experimental

The title α-amino amide, (I), was obtained from a diastereomeric mixture of four α-amino nitriles on treatment with concentrated sulfuric acid for 7 d and subsequent column chromatography on silica gel with petroleum ether (313–333 K)/ethyl acetate (1:3) as eluent. The isolated free base of (I) was then converted into its hydrochloride in ether saturated with HCl gas. Colourless crystals of (I) were obtained from methanol/ether (3:1) [m.p. 480 K; [α] = +7.7° (c = 0.963 g dm^{-3}, MeOH)].

Crystal data

$C_8H_{17}N_2O_2^+\cdot Cl^-\cdot 0.25H_2O$
M_r = 213.19
Orthorhombic
$P2_12_12_1$
a = 11.507 (2) Å
b = 15.225 (5) Å
c = 24.573 (9) Å
V = 4305 (2) Å^3
Z = 16
D_x = 1.316 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 31 034 reflections
θ = 3–26°
μ = 0.330 mm^{-1}
T = 110 (1) K
Prism
0.30 × 0.28 × 0.25 mm
Colourless

Data collection

MAR 180 mm image-plate scanner
Area detector
Absorption correction: none
32 715 measured reflections
4456 independent reflections (plus 3567 Friedel-related reflections)

7962 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.023
$\theta_{\rm max}$ = 25.95°
$h = -13 \rightarrow 13$
$k = -18 \rightarrow 18$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.063
S = 1.056
8023 reflections
575 parameters
H atoms: see below

$(\Delta/\sigma)_{\rm max}$ = 0.002
$\Delta\rho_{\rm max}$ = 0.349 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.161 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 1.0952P]$
where $P = (F_o^2 + 2F_c^2)/3$

Absolute structure: Flack (1983)
Flack parameter = 0.01 (2)

Table 1. *Selected geometric parameters (Å, °)*

N1—C1	1.502 (2)	O12—C17	1.232 (2)
N2—C7	1.325 (2)	N21—C21	1.505 (2)
O1—C8	1.419 (2)	N22—C27	1.331 (2)
O1—C2	1.422 (2)	O22—C27	1.231 (2)
O2—C7	1.230 (2)	N31—C31	1.504 (2)
C1—C7	1.544 (2)	N32—C37	1.325 (2)
N11—C11	1.495 (2)	O32—C37	1.238 (2)
N12—C17	1.327 (2)		
C8—O1—C2	116.3 (1)	O1—C2—C3	106.8 (1)
N1—C1—C7	105.8 (1)	O1—C2—C1	110.4 (1)
N1—C1—C6	110.3 (1)	C3—C2—C1	111.7 (1)
C7—C1—C6	107.95 (11)	O2—C7—N2	124.0 (1)
N1—C1—C2	107.7 (1)	O2—C7—C1	119.4 (1)
C7—C1—C2	113.9 (1)	N2—C7—C1	116.5 (1)
C7—C1—C2—H21	54.7 (10)	C18—O11—C12—C11	156.2 (1)
N1—C1—C2—H21	171.8 (10)	N11—C11—C12—O11	55.1 (1)
C17—C11—C12—H121	54.5 (12)	C17—C11—C12—O11	−60.1 (2)
N11—C11—C12—H121	169.7 (12)	N11—C11—C17—N12	−167.9 (1)
C27—C21—C22—H221	62.6 (11)	C28—O21—C22—C21	168.1 (1)
N21—C21—C22—H221	178.0 (10)	N21—C21—C22—O21	58.8 (1)
C37—C31—C32—H321	55.7 (11)	C27—C21—C22—O21	−56.7 (1)
N31—C31—C32—H321	170.6 (11)	N21—C21—C27—N22	172.7 (1)
C8—O1—C2—C1	82.1 (2)	C38—O31—C32—C31	171.4 (1)
N1—C1—C2—O1	48.7 (1)	N31—C31—C32—O31	52.2 (1)
C7—C1—C2—O1	−68.3 (1)	C37—C31—C32—O31	−62.7 (1)
N1—C1—C7—N2	−172.9 (1)	N31—C31—C37—N32	175.5 (1)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O32	0.85 (2)	2.02 (2)	2.862 (2)	168.9 (1.9)
N1—H1B···Cl2$^{\rm i}$	0.86 (3)	2.32 (2)	3.177 (2)	171.8 (1.7)
N1—H1C···Cl1	0.90 (2)	2.37 (2)	3.222 (2)	156.7 (1.6)
N2—H2A···O22	0.84 (2)	2.16 (2)	2.979 (2)	163.5 (2.0)
N2—H2B···Cl1$^{\rm ii}$	0.73 (2)	2.64 (2)	3.282 (1)	147.8 (2.1)
N11—H11A···O41$^{\rm iii}$	0.90 (2)	1.95 (2)	2.746 (2)	147.5 (1.8)
N11—H11B···Cl2$^{\rm iii}$	0.91 (2)	2.37 (2)	3.136 (2)	142.0 (1.6)
N11—H11C···O2$^{\rm iv}$	0.94 (2)	1.93 (2)	2.763 (2)	147.4 (1.7)
N12—H12B···Cl2	0.85 (2)	2.38 (2)	3.203 (2)	164.8 (1.7)
N21—H21B···O12	0.88 (2)	1.95 (2)	2.791 (2)	159.3 (1.8)
N21—H21A···Cl4$^{\rm v}$	0.93 (2)	2.40 (2)	3.285 (2)	158.5 (1.6)
N21—H21C···Cl3$^{\rm vi}$	0.88 (2)	2.35 (2)	3.219 (2)	170.1 (1.7)
N22—H22A···Cl1$^{\rm ii}$	0.85 (2)	2.54 (2)	3.388 (2)	171.8 (1.7)
N22—H22B···Cl3	0.85 (2)	2.59 (2)	3.430 (2)	169.7 (1.7)
N31—H31B···Cl4$^{\rm vii}$	0.94 (2)	2.22 (2)	3.163 (1)	176.6 (1.8)
N31—H31C···Cl3$^{\rm viii}$	0.87 (2)	2.31 (2)	3.120 (2)	155.1 (1.9)
N32—H32A···Cl4	0.86 (2)	2.50 (2)	3.338 (2)	163.2 (1.8)
N32—H32B···Cl1	0.82 (2)	2.50 (2)	3.300 (2)	163.7 (1.9)
O41—H411···Cl2	0.86 (3)	2.62 (3)	3.283 (2)	135.1 (2.3)
O41—H412···Cl4$^{\rm ix}$	0.89 (3)	2.27 (2)	3.126 (2)	163.3 (2.9)

Symmetry codes: (i) $1+x, y, z$; (ii) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$; (iii) $-x, y-\frac{1}{2}, \frac{3}{2}-z$; (iv) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$; (v) $\frac{1}{2}-x, -y, z-\frac{1}{2}$; (vi) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$; (vii) $\frac{1}{2}+x, \frac{1}{2}-y, 2-z$; (viii) $\frac{1}{2}-x, 1-y, \frac{1}{2}+z$; (ix) $x-\frac{1}{2}, \frac{1}{2}-y, 2-z$.

Data were collected on an IP scanner. There were 199 images, each with 1° oscillation range and 3 min exposure time. The structure was solved by direct methods. All non-H atoms were refined anisotropically. All H atoms bound to C atoms were refined using a riding model, except H21, H121, H221 and H321, which were refined isotropically. H atoms bound to N atoms were refined isotropically with a single displacement parameter for each group of H atoms bound to one N atom. The data are 94.8% complete to 2θ = 52°. The absolute structure was determined by refining an enantiomorph-sensitive parameter (Flack, 1983) using all 3567 Friedel pairs.

Data collection: *XDS*98 (Kabsch, 1993). Cell refinement: *XDS*98. Data reduction: *XDS*98. Program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997). Molecular graphics: *CRYSTAN*88 (Burzlaff & Rothammel, 1988). Software used to prepare material for publication: *SHELXL*97 and local software.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1343). Services for accessing these data are described at the back of the journal.

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Mixed stacking and stoichiometry in a π-molecular complex between fluorene and 1,3,5-trinitrobenzene

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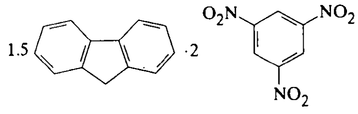
Abstract

The crystal structure of the title complex, fluorene–1,3,5-trinitrobenzene (1.5/2) ($1.5C_{13}H_{10}\cdot 2C_6H_3N_3O_6$) has been determined at room temperature. The molecule crystallizes in a triclinic cell and in the $P\bar{1}$ space group. One of the three fluorene molecules in the unit cell is located at a special position and adopts two different orientations that are related by an inversion center. Therefore, the asymmetric unit contains 1.5 fluorene molecules and two molecules of 1,3,5-trinitrobenzene. Acceptor and donor molecules are arranged in mixed stacks, one with 1:1 and the other with 2:1 trinitrobenzene:fluorene stoichiometries. This mixed arrangement and the composition of the asymmetric unit explains the global 4:3 stoichiometry. These two independent stacking directions are parallel to the *c* and *a* axes, respectively.

Comment

Trinitrobenzolates are charge–transfer compounds formed by donors groups and 1,3,5-trinitrobenzene (TNB) as the acceptor group (Rao, 1970). Usually, these molecular compounds have an integer acceptor–donor ratio, but in this case the observed ratio is 4:3. Herbstein *et al.* (1976) have studied crystals of the fluorene–TNB compound, (I), and reported triclinic yellow plates, $a = 27.63$, $b = 7.563$, $c = 7.264$ Å, $\alpha = 91.2$, $\beta = 92.85$, $\gamma = 98.2°$, $D_x = 1.495\ \mathrm{g\,cm^{-3}}$ and a composition of $(\mathrm{fluorene})_3(\mathrm{TNB})_4$ per unit cell. They suggested that the space group could be $P1$ or $P\bar{1}$, but did not report a structure determination. We have solved the structure and determined that the space group is $P\bar{1}$. There are two independent TNB molecules [(1) and (2)] and two independent fluorene molecules [(3) and (4)] in the asymmetric unit. Fluorene-(4), is situated on a special position and the composition of the asymmetric unit is $(\mathrm{fluorene})_{1.5}(\mathrm{TNB})_2$. The crystal structure also demonstrates that fluorene-(4) is capable of assuming two half-occupied alternative orientations as shown in Fig. 2.



(I)

Both independent fluorene molecules are planar. The maximum absolute deviation from the mean plane is 0.038 (3) Å for C31 and C34 in fluorene-(3) and 0.045 (15) Å for C411 in fluorene-(4). As previously observed (Bar & Bernstein, 1981), the nitro groups belonging to the TNB molecules twist out of the plane of the benzene nucleus. The maximum dihedral angle reported between the least-squares planes of the nitro group and the benzene ring was 15° (Bar & Bernstein, 1981). In the present structure, the maximum angle is 5.0 (3)° for the O13—N12—O14 nitro group of TNB-(1) and 22.5 (2)° for the O21—N21—O22 group of TNB-(2). All bond distances and angles take the expected values for these kinds of compounds.

Fluorene and TNB molecules are arranged in mixed stacks. Two different and independent stacking directions are observed. Each fluorene-(3) molecule packs