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meso-1,2-Diphenylethylenediammonium adipate

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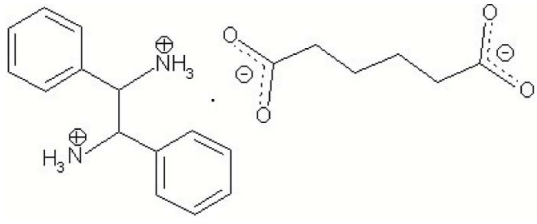
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.061; wR factor = 0.165; data-to-parameter ratio = 19.2.

In the title molecular salt, $C_{14}H_{18}N_2^{2+}\cdot C_6H_8O_4^{2-}$, both the dication and the dianion lie on inversion centers. There is an approximate 61:39 disorder in the central linkage of the cation. In the crystal structure, the components associate *via* N—H···O and C—H···O interactions, resulting in $R_2^2(9)$ rings.

Related literature

For related literature, see: Allen (2002); Bruno *et al.* (2004); Bŭcar *et al.* (2007); Desiraju (1995); Etter (1990); Ferguson *et al.* (1992); Khokhar & Lumetta (1989); Kuroda & Mason (1977); Ramasubramanian *et al.* (2007); Roy *et al.* (2005).



Experimental

Crystal data

$C_{14}H_{18}N_2^{2+}\cdot C_6H_8O_4^{2-}$
M_r = 358.43
Triclinic, $P\overline{1}$
a = 6.361 (3) Å
b = 6.931 (3) Å
c = 11.820 (5) Å
α = 105.35 (2)°
β = 92.05 (2)°
γ = 113.64 (2)°
V = 454.4 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.18 × 0.17 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
8038 measured reflections
2643 independent reflections
1727 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.165
S = 1.03
2643 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H5N···O2^{i}	0.91	1.90	2.769 (2)	159
N1—H6N···O1^{ii}	0.91	1.82	2.717 (2)	167
N1—H3N···O2^{iii}	0.91	1.88	2.756 (2)	161
C6—H6···O2^{ii}	0.95	2.56	3.359 (3)	142
C7—H7···O2^{iv}	0.95	2.53	3.421 (3)	157
C10—H10···O1	0.95	2.42	3.249 (3)	146

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y-1, z$; (iv) $x+1, y-1, z$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The purchase of the diffractometer was made possible by grant No. LEQSF(1999–2000)-ENH-TR-13, administered by the Louisiana Board of Regents.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2481).

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supplementary materials

Acta Cryst. (2007). E**63**, o3800 [**doi:10.1107/S1600536807038937**]

meso-1,2-Diphenylethylenediammonium adipate

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Comment

From the viewpoint of crystal engineering (Desiraju, 1995), adipic acid is a useful species for constructing crystalline architectures because of its proton donating capability to generate hydrogen bonding accepting sites (Roy *et al.*, 2005, Bu˘car *et al.*, 2007), leading to a solid state array with defined dimensionality.

The survey of Khokhar & Lumetta (1989) suggests that *meso*-1,2-diphenylethylenediamine might be useful as a chemotherapeutic agent. This species and its organic and inorganic salts or complexes can develop supramolecular structures by self assembly of components which contain two hydrogen bonding donor sites (Ferguson *et al.*, 1992; Kuroda & Mason, 1977).

As part of our ongoing studies of this species (Ramasubramanian *et al.*,2007), we now report the synthesis and structure of the title compound, (I), (Fig. 1). Double proton transfer from acid to amine has occurred. Both anion and cation are generated by inversion and there is a 61:39 disorder in the central fragment of the cation.

The C—O bond lengths in the adipate moiety indicate delocalization of charge [C—O = 1.244 (1)Å and 1.283 (1) Å] as they are intermediate between single and double bond lengths (Bruno *et al.*, 2004; Allen, 2002).

The species interact by way of N—H···O and C—H···O interactions (Table 1, Fig. 2) such that each cation forms a $R_2^2(9)$ ring (Etter, 1990) with its neighbouring adipate anion. Several other hydrogen-bonded rings are apparent in the crystal packing and they are designated as $R_4^4(28)$, $R_2^3(10)$ $R_2^4(12)$, and $R_2^1(6)$. The $R_4^4(28)$ ring forms an infinite ladder in the crystal by N—H···O interactions (Fig. 3).

Experimental

Stoichiometric quantities of adipic acid and *meso*-1,2-diphenylethylene diamine were separately dissolved in methanol. These solutions were warmed to 343 K and slowly mixed in a 1:1 molar ratio of acid to amine. The resulting mixture was kept at room temperature for slow evaporation of the solvent. Colourless crystals of (I) appeared after two days and were washed with water and dried *in vacuo*.

Refinement

The H atoms were placed in idealized positions (C—H = 0.95–1.00 Å, N—H = 0.91 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(N)$. In the disordered central portion of the cation, the populations of the two conformers [0.613 (8):0.387 (8)] were contrained to sum to unity.

Figures

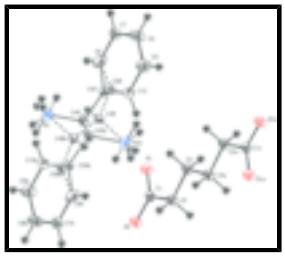

Fig. 1. A view of (I) with displacement ellipsoids shown at the 50% probability level (arbitrary spheres for the H aotms), and only the major orientation of the cation shown. Symmetry codes: (*a*) −*x*, 1 − *y*, −*z*; (*b*) 1 − *x*, 1 − *y*, 1 − *z*.

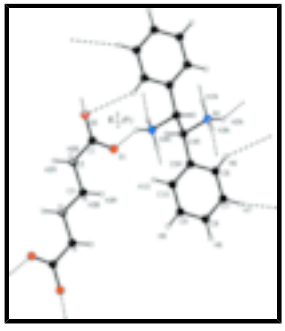

Fig. 2. A view of (I) showing the hydrogen bonds as dashed lines.

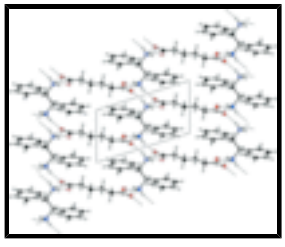

Fig. 3. The hydrogen-bonding interactions of (I) in the crystal packing.

meso-1,2-Diphenylethylenediammonium adipate

Crystal data

$C_{14}H_{18}N_2^{2+}\cdot C_6H_8O_4^{2-}$	$Z = 1$
$M_r = 358.43$	$F_{000} = 192$
Triclinic, $P\overline{1}$	$D_x = 1.310$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.361$ (3) Å	Cell parameters from 2369 reflections
$b = 6.931$ (3) Å	$\theta = 2.5$–30.0º
$c = 11.820$ (5) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 105.35$ (2)º	$T = 100$ K
$\beta = 92.05$ (2)º	Shard, colourless
$\gamma = 113.64$ (2)º	0.18 × 0.17 × 0.15 mm
$V = 454.4$ (4) Å^3	

Data collection

Nonius KappaCCD diffractometer	1727 reflections with $I > 2\sigma(I)$

Radiation source: fine-focus sealed tube	$R_{int} = 0.040$
Monochromator: graphite	$\theta_{max} = 30.1°$
$T = 100$ K	$\theta_{min} = 3.3°$
ω scans with κ offsets	$h = -8 \rightarrow 8$
Absorption correction: none	$k = -9 \rightarrow 9$
8038 measured reflections	$l = -16 \rightarrow 16$
2643 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.061$	$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2 + 0.226P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.165$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
2643 reflections	$\Delta\rho_{min} = -0.35$ e Å^{-3}
138 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.029 (9)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.2968 (2)	0.6691 (2)	0.29572 (11)	0.0219 (3)	
O2	0.0766 (2)	0.8389 (2)	0.37116 (10)	0.0222 (3)	
C1	0.1389 (3)	0.7285 (3)	0.28460 (15)	0.0172 (4)	
C2	0.0067 (3)	0.6698 (3)	0.16156 (15)	0.0189 (4)	
H2A	0.0321	0.8088	0.1441	0.023*	
H2B	−0.1614	0.5914	0.1631	0.023*	
C3	0.0716 (3)	0.5271 (3)	0.06021 (14)	0.0204 (4)	
H3A	0.0472	0.3874	0.0767	0.024*	
H3B	0.2387	0.6055	0.0564	0.024*	

N1	0.3377 (3)	0.2390 (2)	0.54090 (14)	0.0210 (4)	
H1N	0.2729	0.3005	0.5989	0.031*	0.613 (8)
H2N	0.4619	0.2284	0.5746	0.031*	0.613 (8)
H3N	0.2306	0.1017	0.4977	0.031*	0.613 (8)
H4N	0.3499	0.1461	0.4735	0.031*	0.387 (8)
H5N	0.1921	0.1784	0.5588	0.031*	0.387 (8)
H6N	0.4440	0.2603	0.6019	0.031*	0.387 (8)
C4A	0.4175 (5)	0.3837 (5)	0.4595 (3)	0.0162 (9)	0.613 (8)
H4A	0.2786	0.3923	0.4229	0.019*	0.613 (8)
C5A	0.5268 (8)	0.2904 (7)	0.3605 (3)	0.0156 (8)	0.613 (8)
C4B	0.3833 (8)	0.4618 (8)	0.5214 (5)	0.0158 (14)	0.387 (8)
H4B	0.2628	0.4322	0.4545	0.019*	0.387 (8)
C5B	0.6303 (13)	0.3637 (10)	0.3729 (4)	0.0150 (12)	0.387 (8)
C6	0.7312 (4)	0.2447 (3)	0.38574 (18)	0.0350 (5)	
H6	0.8136	0.2963	0.4642	0.042*	
C7	0.7970 (3)	0.1269 (3)	0.29318 (16)	0.0222 (4)	
H7	0.9117	0.0774	0.3076	0.027*	
C8	0.6942 (4)	0.0812 (4)	0.17879 (18)	0.0352 (5)	
H8	0.7372	−0.0020	0.1139	0.042*	
C9	0.5293 (4)	0.1554 (3)	0.15777 (18)	0.0303 (5)	
H9	0.4608	0.1242	0.0785	0.036*	
C10	0.4644 (4)	0.2733 (4)	0.25008 (18)	0.0314 (5)	
H10	0.3718	0.3446	0.2340	0.038*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0225 (7)	0.0251 (7)	0.0179 (6)	0.0129 (6)	0.0003 (5)	0.0023 (5)
O2	0.0251 (7)	0.0265 (7)	0.0134 (6)	0.0137 (6)	0.0021 (5)	−0.0004 (5)
C1	0.0178 (8)	0.0164 (8)	0.0152 (8)	0.0056 (7)	0.0028 (6)	0.0042 (6)
C2	0.0194 (9)	0.0215 (8)	0.0144 (8)	0.0099 (7)	0.0013 (6)	0.0014 (6)
C3	0.0211 (9)	0.0246 (9)	0.0140 (8)	0.0109 (8)	0.0014 (7)	0.0020 (7)
N1	0.0176 (7)	0.0203 (7)	0.0240 (8)	0.0060 (6)	0.0016 (6)	0.0089 (6)
C4A	0.0167 (14)	0.0177 (14)	0.0126 (17)	0.0073 (12)	0.0018 (11)	0.0022 (12)
C5A	0.0159 (19)	0.0112 (16)	0.0156 (15)	0.0046 (14)	0.0025 (14)	−0.0004 (12)
C4B	0.018 (2)	0.019 (2)	0.014 (3)	0.0102 (19)	0.0033 (17)	0.006 (2)
C5B	0.019 (3)	0.012 (3)	0.008 (2)	0.004 (2)	0.002 (2)	−0.0007 (19)
C6	0.0673 (16)	0.0301 (10)	0.0156 (9)	0.0320 (11)	−0.0003 (9)	0.0026 (8)
C7	0.0203 (9)	0.0239 (9)	0.0235 (9)	0.0101 (8)	0.0059 (7)	0.0074 (7)
C8	0.0468 (14)	0.0465 (13)	0.0190 (10)	0.0334 (12)	0.0045 (9)	−0.0013 (9)
C9	0.0374 (12)	0.0315 (11)	0.0199 (9)	0.0199 (10)	−0.0031 (8)	−0.0029 (8)
C10	0.0459 (13)	0.0395 (11)	0.0295 (11)	0.0319 (11)	0.0193 (9)	0.0196 (9)

Geometric parameters (Å, °)

O1—C1	1.244 (2)	C4A—H4A	1.0000
O2—C1	1.283 (2)	C5A—C10	1.311 (4)
C1—C2	1.521 (2)	C5A—C6	1.494 (4)

C2—C3	1.523 (2)	C4B—C4B^{ii}	1.518 (9)
C2—H2A	0.9900	C4B—C5B^{ii}	1.524 (8)
C2—H2B	0.9900	C4B—H4B	1.0000
C3—C3^{i}	1.532 (3)	C5B—C6	1.264 (6)
C3—H3A	0.9900	C5B—C4B^{ii}	1.524 (8)
C3—H3B	0.9900	C5B—C10	1.579 (6)
N1—C4A	1.525 (3)	C6—C7	1.368 (3)
N1—C4B	1.535 (5)	C6—H6	0.9500
N1—H1N	0.9100	C7—C8	1.378 (3)
N1—H2N	0.9100	C7—H7	0.9500
N1—H3N	0.9100	C8—C9	1.382 (3)
N1—H4N	0.9100	C8—H8	0.9500
N1—H5N	0.9100	C9—C10	1.364 (3)
N1—H6N	0.9100	C9—H9	0.9500
C4A—C5A	1.513 (5)	C10—H10	0.9500
C4A—C4A^{ii}	1.540 (6)		
O1—C1—O2	124.40 (16)	C4A^{ii}—C4A—H4A	108.3
O1—C1—C2	119.49 (15)	C10—C5A—C6	117.1 (3)
O2—C1—C2	116.11 (15)	C10—C5A—C4A	120.7 (3)
C1—C2—C3	115.80 (15)	C6—C5A—C4A	121.6 (3)
C1—C2—H2A	108.3	C4B^{ii}—C4B—C5B^{ii}	112.9 (6)
C3—C2—H2A	108.3	C4B^{ii}—C4B—N1	106.0 (5)
C1—C2—H2B	108.3	C5B^{ii}—C4B—N1	115.8 (4)
C3—C2—H2B	108.3	C4B^{ii}—C4B—H4B	107.2
H2A—C2—H2B	107.4	C5B^{ii}—C4B—H4B	107.2
C2—C3—C3^{i}	112.47 (18)	N1—C4B—H4B	107.2
C2—C3—H3A	109.1	C6—C5B—C4B^{ii}	121.6 (4)
C3^{i}—C3—H3A	109.1	C6—C5B—C10	114.3 (4)
C2—C3—H3B	109.1	C4B^{ii}—C5B—C10	122.0 (4)
C3^{i}—C3—H3B	109.1	C5B—C6—C7	123.0 (3)
H3A—C3—H3B	107.8	C7—C6—C5A	118.5 (2)
C4A—N1—H1N	109.5	C5B—C6—H6	110.9
C4A—N1—H2N	109.5	C7—C6—H6	120.8
H1N—N1—H2N	109.5	C5A—C6—H6	120.8
C4A—N1—H3N	109.5	C6—C7—C8	119.01 (18)
H1N—N1—H3N	109.5	C6—C7—H7	120.5
H2N—N1—H3N	109.5	C8—C7—H7	120.5
C4B—N1—H4N	109.5	C7—C8—C9	120.51 (18)
C4B—N1—H5N	109.5	C7—C8—H8	119.7
H4N—N1—H5N	109.5	C9—C8—H8	119.7
C4B—N1—H6N	109.5	C10—C9—C8	120.41 (19)
H4N—N1—H6N	109.5	C10—C9—H9	119.8
H5N—N1—H6N	109.5	C8—C9—H9	119.8
C5A—C4A—N1	112.2 (2)	C5A—C10—C9	121.5 (2)
C5A—C4A—C4A^{ii}	113.4 (4)	C9—C10—C5B	114.8 (3)

N1—C4A—C4A^{ii}	106.2 (3)	C5A—C10—H10	119.3
C5A—C4A—H4A	108.3	C9—C10—H10	119.3
N1—C4A—H4A	108.3	C5B—C10—H10	120.9
O1—C1—C2—C3	3.6 (2)	C10—C5A—C6—C7	−19.3 (5)
O2—C1—C2—C3	−176.46 (15)	C4A—C5A—C6—C7	169.2 (3)
C1—C2—C3—C3^{i}	179.22 (19)	C5B—C6—C7—C8	−19.5 (5)
C4B—N1—C4A—C5A	168.8 (5)	C5A—C6—C7—C8	8.8 (4)
C4B—N1—C4A—C4A^{ii}	44.4 (4)	C6—C7—C8—C9	0.8 (3)
N1—C4A—C5A—C10	131.7 (3)	C7—C8—C9—C10	−0.6 (4)
C4A^{ii}—C4A—C5A—C10	−108.0 (4)	C6—C5A—C10—C9	20.1 (5)
N1—C4A—C5A—C6	−57.1 (4)	C4A—C5A—C10—C9	−168.3 (3)
C4A^{ii}—C4A—C5A—C6	63.2 (5)	C6—C5A—C10—C5B	−59.2 (7)
C4A—N1—C4B—C4B^{ii}	−45.1 (4)	C4A—C5A—C10—C5B	112.4 (8)
C4A—N1—C4B—C5B^{ii}	−171.2 (6)	C8—C9—C10—C5A	−10.8 (4)
C4B^{ii}—C5B—C6—C7	−163.5 (4)	C8—C9—C10—C5B	14.2 (4)
C10—C5B—C6—C7	32.9 (7)	C6—C5B—C10—C5A	82.6 (8)
C4B^{ii}—C5B—C6—C5A	109.4 (10)	C4B^{ii}—C5B—C10—C5A	−80.8 (8)
C10—C5B—C6—C5A	−54.1 (6)	C6—C5B—C10—C9	−30.0 (6)
C10—C5A—C6—C5B	88.3 (8)	C4B^{ii}—C5B—C10—C9	166.5 (4)
C4A—C5A—C6—C5B	−83.2 (7)		

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H5N···O2^{iii}	0.91	1.90	2.769 (2)	159
N1—H6N···O1^{ii}	0.91	1.82	2.717 (2)	167
N1—H3N···O2^{iv}	0.91	1.88	2.756 (2)	161
C6—H6···O2^{ii}	0.95	2.56	3.359 (3)	142
C7—H7···O2^{v}	0.95	2.53	3.421 (3)	157
C10—H10···O1	0.95	2.42	3.249 (3)	146

Symmetry codes: (iii) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*, *y*−1, *z*; (v) *x*+1, *y*−1, *z*.

Fig. 1

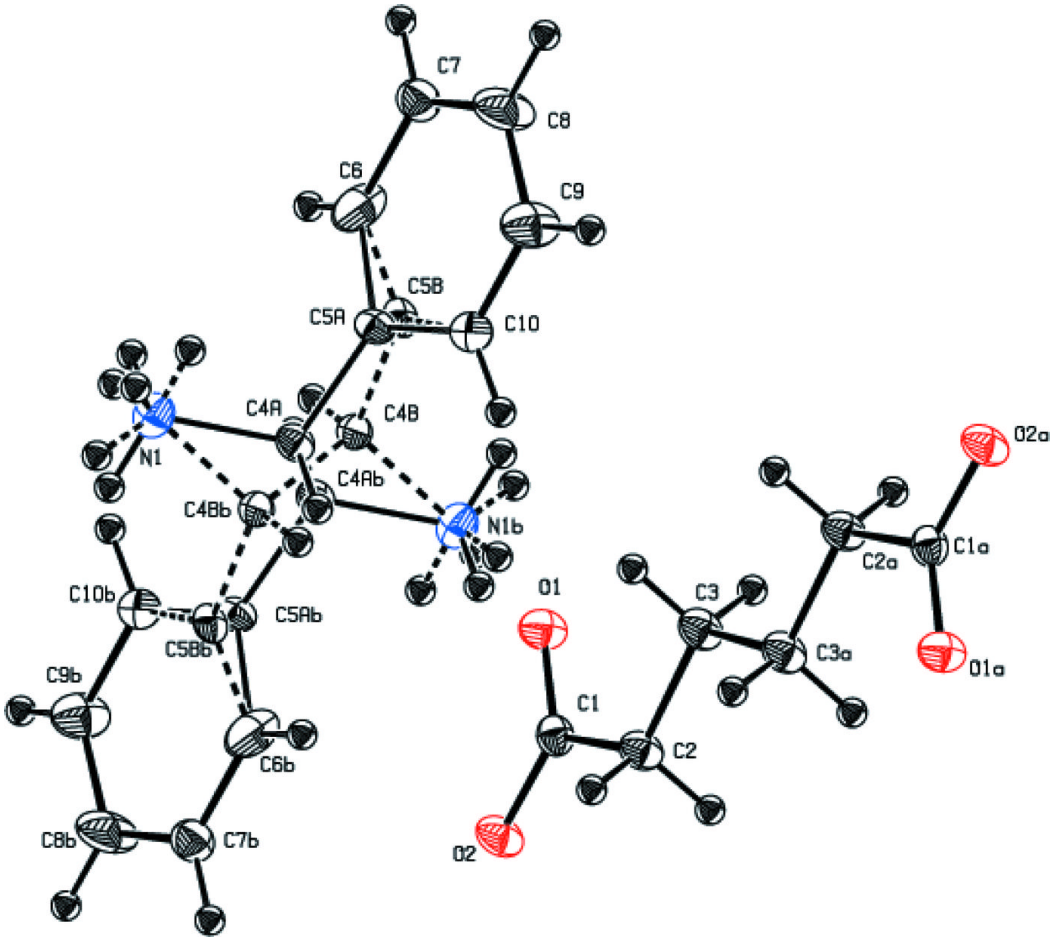
C7
C8
C6
C9
C5B
C5A
C10
C4A
C4B
N1
C4Ab
C4Bb
N1b
C10b
C5Ab
C5Bb
C9b
C6b
C8b
C7b
O1
C1
C2
O2
C3
C3a
C2a
C1a
O2a
O1a

Fig. 2

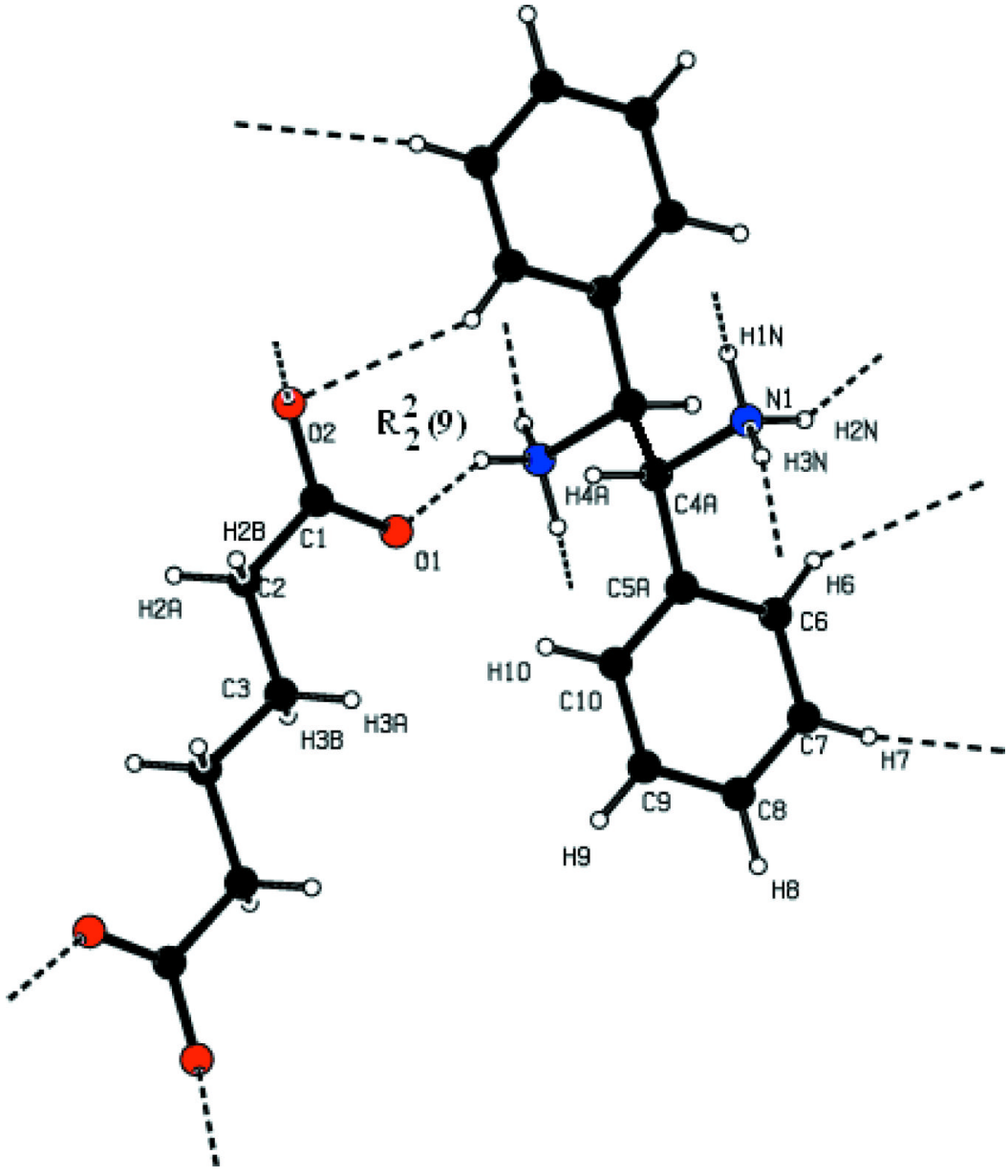
H1N
N1
H2N
H3N
O2
$R_2^2(9)$
H4A
C4A
H2B
C1
O1
C2
H2A
C5A
H6
C6
H10
C10
C3
H3A
H3B
C7
H7
C9
C8
H9
H8

Fig. 3