Low-dimensional hydrogen-bonded structures in the 1:1 and 1:2 proton-transfer compounds of 4,5-dichlorophthalic acid with the aliphatic Lewis bases triethylamine, diethylamine, n-butylamine and piperidine

Author
Smith, Graham, Wermuth, Urs

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Graham Smith and Urs D. Wermuth

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Graham Smitha and Urs D. Wermuthb

aFaculty of Science and Technology, Queensland University of Technology, GPO Box 2434, Brisbane, Queensland 4001, Australia, and bSchool of Biomolecular and Physical Sciences, Griffith University, Nathan, Queensland 4111, Australia

Correspondence e-mail: g.smith@qut.edu.au

The structures of the proton-transfer compounds of 4,5-dichlorophthalic acid (DCPA) with the aliphatic Lewis bases triethylamine, diethylamine, n-butylamine and piperidine, namely triethylaminium 2-carboxy-4,5-dichlorobenzoate, C6H3N+·C8H7Cl2O4−, (I), diethylaminium 2-carboxy-4,5-dichlorobenzoate, C6H12N+·C8H7Cl2O4−, (II), bis(butanaminium) 4,5-dichlorobenzene-1,2-dicarboxylate monohydrate, 2C4H12N+·C8H3Cl2O4·H2O, (III), and bis(piperidinium) 4,5-dichlorobenzene-1,2-dicarboxylate monohydrate, 2C6H12N+·C8H3Cl2O4·H2O, (IV), have been determined at 200 K. All compounds have hydrogen-bonding associations, giving discrete cation–anion units in (I) and linear chains in (II), while (III) and (IV) both have two-dimensional structures. In (I), a discrete cation–anion unit is formed through an asymmetric R2(4) N+–H···O2 hydrogen-bonding association, whereas in (II), chains are formed through linear N–H···O associations involving both aminium H-atom donors. In compounds (III) and (IV), the primary N–H···O-linked cation–anion units are extended into a two-dimensional sheet structure via amide–carboxyl N–H···O and amide–carbonyl N–H···O interactions. In the 1:1 salts (I) and (II), the hydrogen 4,5-dichlorophthalate anions are essentially planar with short intramolecular carboxyl–carbonyl O–H···O hydrogen bonds [O···O = 2.4223 (14) and 2.388 (2) Å, respectively]. This work provides a further example of the uncommon zero-dimensional hydrogen-bonded DCPA–Lewis base salt and the one-dimensional chain structure type, while even with the hydrate structures of the 1:2 salts with the primary and secondary amines, the low dimensionality generally associated with 1:1 DCPA salts is also found.

The 1:1 examples with the secondary aliphatic amine diisopropylamine and the tertiary amine hexamethylenetetramine (Smith & Wermuth, 2010a) show simple one-dimensional hydrogen-bonded chain structures. Hydrates are also uncommon among the structures of the 1:1 proton-transfer compounds of DCPA, which is unusual considering that their common preparation is in aqueous alcoholic solution, or they are recrystallized from water, as is the case with the four compounds reported here. The only five known hydrated examples are the ammonium salt (Mattes & Dorau, 1986) (a monohydrate) and the salts with quinaldic acid (a monohydrate; Smith et al., 2008a), 2-aminobenzoic acid (a dihydrate; Smith et al., 2008b), hexamethylenetetramine (a monohydrate; Smith & Wermuth, 2010a) and the salt of the

Comment

The proton-transfer compounds of the acid salts of 4,5-dichlorophthalic acid (DCPA) with aromatic and heteroaromatic nitrogen Lewis bases generally show low-dimensional hydrogen-bonded structure types (Smith et al., 2008a, 2009a), with the occurrence of three-dimensional structures limited to the salts with the bifunctional associative-group-substituted compounds 3- and 4-aminobenzoic acid (Smith et al., 2008b) and 4-chloroaniline (Smith et al., 2009b). In two of these examples (with the aminocarboxylic acids), the primary hydrogen-bonded cation–anion ‘heterodimers’ (Etter & Adsmond, 1990) are extended into sheet substructures then into three-dimensional framework structures through cation associative-substituent-group interactions. In these three-dimensional structures, the DCPA anions are nonplanar (the ‘nonplanar’ conformation), whereas in the low-dimensional structure types the DCPA anion species are essentially planar (the ‘planar’ conformation) with the planarity a consequence of the short intramolecular carboxyl–carbonyl O–H···O hydrogen bond [typically 2.4054 (19) Å in the 1:1 1,10-phenanthroline–DCPA salt (Smith et al., 2009c)].
drug quinacrine (a tetrahydrate; Smith et al., 2009). The dianionic DCPA anion is similarly uncommon among the known structures, examples being the salts with 4-ethylaniline (Odabasoğlu & Büyükgüngör, 2007) and ethylenediamine (Smith & Wermuth, 2010c). It has been previously noted (Smith et al., 2009c) in the structure of the 1,10-phenanthroline salt that with the ‘planar’ DCPA cations, there is a common set of abnormal bond parameters associated with the intramolecular hydrogen-bonded unit which typically evoke level C alerts in checkCIF (Spek, 2009), viz. significant bond lengthening of the \( \text{exo-C1} - \text{C}_{\text{carboxyl}} \) and \( \text{exo-C2} - \text{C}_{\text{carboxyl}} \) bonds, together with distortion of the external aromatic ring C to carboxyl C bond angles. It was intended in this work that, together with a description of the hydrogen-bonding features of four new DCPA salts, we would examine the complete set of known ‘planar’ hydrogen DCPA structures and compare these abnormal but interrelated features.

Because the known structures of the 1:1 aliphatic Lewis base salts with DCPA, with the exception of the ammonium salt (Mattes & Dorau, 1986), invariably have the ‘planar’ anion and since the number of characterized aliphatic examples is not great, we carried out the 1:1 stoichiometric reaction of DCPA with a series of aliphatic amines. Our experience indicated that such preparations generally yielded noncrystalline powders from methanol solution (a solvent of choice for the aromatic salts), but if recrystallized from water, they often gave crystals suitable for X-ray analysis. Using this technique, small quantities were obtained of quality crystals of the DCPA salts of the primary amine \( n \)-butylamine, the secondary amines diethylamine and piperidine and the tertiary amine triethylamine. These compounds are anhydrous triethylammonium 2-carboxy-4,5-dichlorobenzoate, (I), diethylaminium 2-carboxy-4,5-dichlorobenzoate, (II), and the hydrated salts bis(butanaminium) 4,5-dichlorobenzene-1,2-dicarboxylate monohydrate, (III), and bis(piperidinium) 4,5-dichlorobenzene-1,2-dicarboxylate monohydrate, (IV), and the structures are reported here (Figs. 1–4).

**Figure 1**
The molecular configuration and atom-numbering scheme for the triethylammonium cation and the 2-carboxy-4,5-dichlorobenzoate anion in (I). Non-H atoms are shown as 40% probability displacement ellipsoids.

**Figure 2**
The molecular configuration and atom-numbering scheme for the isopropylaminium cation and the 2-carboxy-4,5-dichlorobenzoate anion in (II). Non-H atoms are shown as 40% probability displacement ellipsoids.

**Figure 3**
The molecular configuration and atom-numbering scheme for the two \( n \)-butylaminium cations (A and B), the 4,5-dichlorophthalate dianion and the water molecule of solvation (O1W) in (III). Inter- and intra-species hydrogen bonds are shown as dashed lines and non-H atoms are shown as 40% probability displacement ellipsoids.

**Figure 4**
The molecular configuration and atom-numbering scheme for the two piperidinium cations (A and B), the 4,5-dichlorophthalate dianion and the water molecule of solvation (O1W) in (IV). Non-H atoms are shown as 40% probability displacement ellipsoids.
Considering the 1:1 stoichiometric reaction conditions employed in the preparation of all four compounds, which should have resulted in 1:1 salts, compounds (III) and (IV) are unusual, giving dianionic phthalate salts as well as being hydrates, whereas (I) and (II) are the expected and more common anhydrous 1:1 hydrogen phthalate salts. All members of this set of compounds show low-dimensional hydrogen-bonded structures: zero- in (I), one- in (II) and two-dimensional in (III) and (IV) (Figs. 5–8). Also, all have at least one \( N^+\!-\!H\cdots O \) carboxyl hydrogen-bonding interaction (Figs. 1–4), (II) having two such interactions, but in compounds (III) and (IV), the water O atom acts as an acceptor in an \( N^+\!-\!H\cdots O \) hydrogen bond (Tables 1–4). A listing of significant structural parameters for the DCPA anions of (I) and (II), as well as those for the complete set of ‘planar’ DCPA salts, is also made (Table 5).

With compound (I) the only cation–anion hydrogen-bonding association is asymmetric cyclic, involving both carboxyl O-atom acceptors [graph set \( R_2^1(4) \); Etter et al., 1990] (Table 1). This results in discrete cation–anion units (‘heterodimers’; Etter & Adsmond, 1990), giving a zero-dimensional structure (Fig. 1). This structure therefore represents only the fifth of its type among the known series of 1:1 DCPA salts, the others being the tetra-\( n \)-butylammonium salt (Mattes & Dorau, 1986), the 1,8-bis(dimethylamino)naphthalene salt (Mallinson et al., 2003; Parkin et al., 2007), the brucinium salt (Smith et al., 2007) and the 1,10-phenanthroline salt (Smith et al., 2009a), although the tetramethylammonium salt of DCPA (Bozkurt et al., 2006) may also be considered discrete on the basis of formal intermolecular \( N^+\!-\!H\cdots O \) hydrogen bonds. A unique discrete ‘heterotetramer’ (Etter & Adsmond, 1990) is found in the 1:1 compound with 2-aminopyrimidine (Smith et al., 2009a). The only intermolecular associations in the structure of (I) are weak anion–anion \( \pi\!-\!\pi \) interactions [ring centroid separation = 3.6494 (8) \( \AA \)] due to partial aromatic ring overlap down the \( a \)
groups and B bridging a carboxyl group and a water O-atom acceptor. The water also bridges carboxyl groups giving much larger conjoint cyclic interactions [graph sets $R_6^2(18)$ and $R_6^2(17)$] (Table 4). Duplex chains which lie along the c cell direction are extended down the b direction giving a two-dimensional sheet structure (Fig. 9). The conformations of the two carboxyl groups in the ‘nonplanar’ DCPA dianions in (III) and (IV) differ but not significantly [torsion angles $C1–C2–C21–O22$ and $C2–C1–C11–O11$ are, respectively, 147.29 (15) and 125.00 (17)° for (III), and $-141.41$ (13) and $-118.74$ (15)° for (IV)] since these values would be expected to be affected by hydrogen-bonding environments.

There is an absence in (I)–(IV) of short intermolecular Cl−•••Cl interactions such as has been found in the 1:1 DCPA compounds with the 3- and 4-aminobenzoic acids (Smith et al., 2008a). However, in one of the ‘planar’ structures, (II), there are short intermolecular Cl−•••O_carboxyl associations [Cl4−•••O22ii = 2.9769 (17) Å; symmetry code: (ii) $-x + 1, y - \frac{1}{2}, z$].

With the ‘planar’ DCPA monoanions which comprise 19 of the total of 26 known examples within the series of known 1:1 compounds with both aromatic and aliphatic amines, there are also other inherent structural features which are present, including some which evoke checkCIF C alerts, as follows: (i) long $sp^2$–$sp^2$ C_neighbor–C_carboxyl bond distances; (ii) distortion of the external bond angles associated with the C−C_carboxyl bonds; (iii) short aromatic C3−$sp^2$–O_carboxyl and C6−H−•••O_carboxyl interactions. However, with point (iii), these short C−O contacts [2.6714 (16) and 2.6602 (17) Å for (I), and 2.663 (3) and 2.662 (2) Å for (II)] are artefacts of the ‘planar’ anion conformation. Table 5 lists the values relating to points (i) and (ii) for (I) and (II), as well as the comparative values for the intramolecular O−H−•••O carboxyl hydrogen bonds and the associated C2−C1−C11−O11 and C1−C2−C21−O22 torsion angles for the full set of known 1:1 ‘planar’ DCPA compounds, and a remarkable consistency is observed. Regarding point (i), the lengthening of the C1−C11 and C2−C21 bonds [1.5366 (19) and 1.5344 (19) Å in (I), and 1.530 (3) and 1.521 (3) Å in (II)] compares with the bond-length range: 1.511 (6) Å in the quinacrine salt (Smith et al., 2009) to 1.538 (3) Å in the 1,10-phenanthroline salt (Smith et al., 2009c). A typical value for this bond in a ‘nonplanar’ example is 1.500 (2) Å in the 2-carboxyaminilumium–DCPA salt (Smith et al., 2008b). Regarding point (ii), the exo-C1 and C2 ring angles [C1−C2−C21 and C2−C1−C11] [128.16 (11) and 129.73 (11)° for (I), and 128.33 (17) and 128.49 (16)° in (II)] compare with the range of 127.88 (16)° in the nicotaminide salt (Smith et al., 2008a) to 129.73 (11)° in compound (I). The distances for the intramolecular hydrogen bond range from 2.34 (1) Å in the tetra-n-butylammonium salt (Mates & Dorau, 1986) to 2.4507 (16) Å in the isopropylamine salt (Smith & Wermuth, 2010b), the latter being associated with the maximum deviation from planarity in the series, indicated by the C2−C1−C11−O11 torsion angle of $-156.69$ (13)°

Considering the high incidence of the ‘planar’ monoanionic DCPA species among this set of salts, it is apparent that the structural distortions invariably present in the anion, which
are a consequence of the internal carboxyl hydrogen bond, are accommodated internally rather than by assuming the ‘nonplanar’ conformation.

This present series of salts provides further examples of low-dimensional hydrogen-bonded structure types in the series of both 1:1 and 1:2 proton-transfer compounds of 4,5-dichlorophthalic acid with aliphatic Lewis bases. The dimensionality of the structure should be largely dictated by the type of amine involved (primary, secondary or tertiary), but with the 1:1 examples, the ‘planar’ internally hydrogen-bonded hydrogen phthalate anion species is found and with it low-dimensional hydrogen-bonded structures. This is also the case with the ‘nonplanar’ 1:2 dianionic DCPA examples, (III) and (IV). Furthermore, there is little variation in the conformational features of the monoanionic ‘planar’ DCPA anion species.

Experimental

Compounds (I)–(IV) were synthesized by heating together for 10 min under reflux 1 mmol quantities of 4,5-dichlorophthalic acid and, respectively, triethylamine, diethylamine, n-butylamine and piperidine in methanol (50 ml). All preparations gave colourless powders on complete evaporation of solvent but subsequent recrystallization from water gave, in all cases, small quantities of colourless crystals suitable for X-ray analysis [m.p.: 353 K in (I), 443 K in (II), 405 K in (III) and 447 K in (IV)].

**Compound (I)**

**Crystal data**

C$_6$H$_{16}$N+$\cdot$C$_9$H$_{16}$Cl$_2$O$_4$ $-$  
$M_r$ = 336.20  
Monoclinic, $P2_1/c$  
$a = 7.3206$ (7) Å  
b = 11.2201 (7) Å  
c = 19.4813 (12) Å  
$\beta = 98.576$ (7)$^\circ$

**Data collection**

Oxford Diffraction Gemini-S CCD-diffractometer  
Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)  
$T_{\text{min}}$ = 0.96, $T_{\text{max}}$ = 0.98

10740 measured reflections  
5298 independent reflections  
2638 reflections with $I > 2\sigma(I)$  
$R_{\text{int}}$ = 0.020

**Refinement**

$R[F^2 > 2\sigma(F^2)] = 0.029$  
w$R(F) = 0.077$  
$S = 1.04$  
3639 reflections  
193 parameters

H atoms treated by a mixture of independent and constrained refinement  
$\Delta \rho_{\text{max}} = 0.23$ e Å$^{-3}$  
$\Delta \rho_{\text{min}} = -0.24$ e Å$^{-3}$

**Compound (II)**

**Crystal data**

C$_{20}$H$_{22}$N$_2$$-$$\cdot$C$_9$H$_{16}$Cl$_2$O$_4$$-$$\cdot$H$_2$O  
$M_r$ = 399.30  
Monoclinic, $P2_1/c$  
a = 8.1362 (6) Å  
b = 9.3043 (11) Å  
c = 15.406 (1) Å  
$\beta = 85.846$ (6)$^\circ$

**Data collection**

Oxford Diffraction Gemini-S CCD-diffractometer  
Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)  
$T_{\text{min}}$ = 0.865, $T_{\text{max}}$ = 0.940

**Table 1**

Hydrogen-bond geometry (Å, $^\circ$) for (I).

<table>
<thead>
<tr>
<th>D–H $\cdot$–A</th>
<th>D–H</th>
<th>H $\cdot$–A</th>
<th>D $\cdot$–A</th>
<th>D–H $\cdot$–A</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1A–H1A$\cdot$–O21</td>
<td>0.91 (15)</td>
<td>1.83 (15)</td>
<td>2.569 (15)</td>
<td>3.164 (15)</td>
</tr>
<tr>
<td>N1A–H1A$\cdot$–O22</td>
<td>0.91 (15)</td>
<td>1.83 (15)</td>
<td>2.569 (15)</td>
<td>3.164 (15)</td>
</tr>
<tr>
<td>O12–H12$\cdot$–O21</td>
<td>0.99 (2)</td>
<td>1.44 (2)</td>
<td>2.4223 (14)</td>
<td>2.4223 (14)</td>
</tr>
</tbody>
</table>

**Table 2**

Hydrogen-bond geometry (Å, $^\circ$) for (II).

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<thead>
<tr>
<th>D–H $\cdot$–A</th>
<th>D–H</th>
<th>H $\cdot$–A</th>
<th>D $\cdot$–A</th>
<th>D–H $\cdot$–A</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1A–H1A$\cdot$–O11$^\text{i}$</td>
<td>0.85 (2)</td>
<td>1.89 (2)</td>
<td>2.772 (2)</td>
<td>169.6 (19)</td>
</tr>
<tr>
<td>N1A–H2A$\cdot$–O22</td>
<td>0.94 (3)</td>
<td>1.83 (3)</td>
<td>2.765 (3)</td>
<td>173 (3)</td>
</tr>
<tr>
<td>O12–H12$\cdot$–O21</td>
<td>0.99 (3)</td>
<td>1.40 (3)</td>
<td>2.388 (2)</td>
<td>179.4 (19)</td>
</tr>
</tbody>
</table>

**Table 3**

Hydrogen-bond geometry (Å, $^\circ$) for (III).

<table>
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<tr>
<th>D–H $\cdot$–A</th>
<th>D–H</th>
<th>H $\cdot$–A</th>
<th>D $\cdot$–A</th>
<th>D–H $\cdot$–A</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1A–H1A$\cdot$–O21</td>
<td>0.88 (2)</td>
<td>1.89 (2)</td>
<td>2.762 (2)</td>
<td>170 (2)</td>
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<tr>
<td>N1A–H1A$\cdot$–O1W$^\text{a}$</td>
<td>0.91 (2)</td>
<td>1.89 (2)</td>
<td>2.762 (2)</td>
<td>170 (2)</td>
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<tr>
<td>N1A–H1A$\cdot$–O21</td>
<td>0.94 (2)</td>
<td>1.94 (2)</td>
<td>2.831 (2)</td>
<td>158.4 (17)</td>
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<tr>
<td>N1B–H1B$\cdot$–O22</td>
<td>0.89 (2)</td>
<td>2.00 (3)</td>
<td>2.847 (2)</td>
<td>158.9 (19)</td>
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<td>N1B–H1B$\cdot$–O21$^\text{a}$</td>
<td>0.89 (3)</td>
<td>1.90 (3)</td>
<td>2.773 (17)</td>
<td>167.9 (17)</td>
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<tr>
<td>N1B–H3B$\cdot$–O1W$^\text{a}$</td>
<td>0.89 (3)</td>
<td>1.86 (3)</td>
<td>2.748 (17)</td>
<td>170 (2)</td>
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<tr>
<td>O1W–H1W$\cdot$–O12</td>
<td>0.85 (3)</td>
<td>1.84 (3)</td>
<td>2.723 (2)</td>
<td>173 (2)</td>
</tr>
<tr>
<td>O1W–H2W$\cdot$–O22$^\text{a}$</td>
<td>0.91 (3)</td>
<td>1.87 (3)</td>
<td>2.755 (18)</td>
<td>166 (3)</td>
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</table>

**Data collection**

Oxford Diffraction Gemini-S CCD-diffractometer  
Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)  
$T_{\text{min}}$ = 0.926, $T_{\text{max}}$ = 0.980

$R_{\text{int}}$ = 0.022

**Refinement**

$R[F^2 > 2\sigma(F^2)] = 0.037$  
wR($F^2$) = 0.106  
$S = 1.05$  
2802 reflections  
184 parameters

H atoms treated by a mixture of independent and constrained refinement  
$\Delta \rho_{\text{max}} = 0.38$ e Å$^{-3}$  
$\Delta \rho_{\text{min}} = -0.26$ e Å$^{-3}$
Table 4
Hydrogen-bond geometry (Å, °) for (IV).

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<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D···H</th>
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<tbody>
<tr>
<td>N1A—H11A···O2I</td>
<td>0.90 (2)</td>
<td>1.80 (2)</td>
<td>2.6820 (17)</td>
<td>164.0 (17)</td>
</tr>
<tr>
<td>N1A—H12A···O11</td>
<td>0.914 (19)</td>
<td>1.907 (19)</td>
<td>2.8085 (17)</td>
<td>186.4 (16)</td>
</tr>
<tr>
<td>N1B—H11B···O1W</td>
<td>0.896 (17)</td>
<td>1.917 (17)</td>
<td>2.8054 (16)</td>
<td>170.7 (16)</td>
</tr>
<tr>
<td>OW···H11W···O12</td>
<td>0.82 (2)</td>
<td>1.93 (2)</td>
<td>2.7490 (17)</td>
<td>176 (2)</td>
</tr>
<tr>
<td>OW···H12W···O2II</td>
<td>0.84 (2)</td>
<td>1.96 (2)</td>
<td>2.7639 (17)</td>
<td>162 (2)</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) −x, y − 1/2, −z + 1; (ii) −x, y + 2, −z.

Refinement

R[F² > 2σ(F²)] = 0.046
wR(F²) = 0.145
S = 1.18
4851 reflections
260 parameters

H atoms treated by a mixture of independent and constrained refinement

Δρ_{max} = 0.41 e Å⁻³
Δρ_{min} = −0.29 e Å⁻³

Compound (IV)

Crystal data

2C₄H₆N₂O₃C₆H₅Cl₂O₄−H₂O
Mr = 423.32
Monoclinic, P2₁/c
a = 13.8481 (10) Å
b = 10.5937 (8) Å
c = 14.6129 (10) Å
β = 99.903 (7)°

Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
T_{min} = 0.701, T_{max} = 0.980
26626 measured reflections
4805 independent reflections
3570 reflections with T > 2σ(I)
R_{int} = 0.057

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD3347). Services for accessing these data are described at the back of the journal.

Table 5
Comparative structural parameters (Å, °) and structural classification for the series of ‘planar’ 1:1 DCPA salts of the named Lewis base types.

<table>
<thead>
<tr>
<th>Lewis base type</th>
<th>Structure type</th>
<th>C1—C11</th>
<th>C2—C21</th>
<th>C1—C2—C21</th>
<th>C2—C1—C11</th>
<th>O12—O21</th>
<th>O12—C21</th>
<th>C2—C1—C11</th>
<th>O12—O21</th>
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<tbody>
<tr>
<td>TEA⁺</td>
<td>0</td>
<td>1.536 (19)</td>
<td>1.534 (19)</td>
<td>128.16 (11)</td>
<td>129.73 (11)</td>
<td>2.4233 (14)</td>
<td>178.46 (13)</td>
<td>176.6 (2)</td>
<td>171.3 (2)</td>
</tr>
<tr>
<td>DEA⁺</td>
<td>2</td>
<td>1.530 (3)</td>
<td>1.523 (3)</td>
<td>128.33 (17)</td>
<td>128.49 (16)</td>
<td>2.388 (2)</td>
<td>−172.41 (19)</td>
<td>175.50 (19)</td>
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<tr>
<td>IPA⁺</td>
<td>1</td>
<td>1.519 (18)</td>
<td>1.529 (18)</td>
<td>128.32 (11)</td>
<td>128.14 (11)</td>
<td>2.450 (16)</td>
<td>161.01 (13)</td>
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<tr>
<td>DIPA⁺</td>
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(1) This work (TEA is triethylamine and DEA is diethylamine); (2) Smith & Wermuth (2010a) (IPA is isopropylamine); (3) Smith & Wermuth (2010a) (DIPA is diisopropylamine and HMT is hexamethylenetetramine); (4) Smith & Wermuth (2010a) (INIPA is isonicotinamide); (4) Smith & Wermuth (2010a) (INICA is nicotinamide, INICA is isonicotinamide and AMPM is 2-aminopyrimidine); (6) Smith & Wermuth (2010a); (7) Smith & Wermuth (2010a) (MPMY is 4-methylpyridine); (8) Smith & Wermuth (2010a) (8-AQ is 8-quinonemine and 8-HQ is 8-hydroquinone); (9) Smith & Wermuth (2010a) (QAC is quinicaine). ① For the quinicaine salt, there are two independent DCPA anions in the asymmetric unit.

Organic compounds


Smith and Wermuth • Four C₄H₆Cl₂O₄⁻ salts
References