**Crystal Structure of 2,6-Diethylphenylammonium Chloride**

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The title compound, \([2,6-(C_6H_5)C_6H_3NH_3]Cl\), crystallizes in the monoclinic space group \(P2_1/a\) with \(a = 8.633(2)\, \text{Å}, b = 20.530(2)\, \text{Å}, c = 12.129(2)\, \text{Å}, \beta = 90.48(2)^\circ\) and \(V = 2149.4(6)\, \text{Å}^3\). The atomic arrangement can be described as corrugated ribbons, containing ammonium groups of the organic cations and chloride anions. As well as electrostatic and van der Walls interactions, the component species interact through multiple hydrogen bonds.

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Organic-inorganic hybrid materials have attracted increasing attention, especially when they are obtained by an appropriate choice of cation and anion. In the last few years, a considerable strategy has been employed in crystal engineering: to take advantage of hydrogen-bond interactions. Indeed, hydrogen bonds have been recognized as being the most powerful force to generate interesting supramolecular networks in one, two and three dimensions.\(^2\,3\) As a part of our continuing interest in this field, we have synthesized a new compound, 2,6-diethylphenylammonium chloride (Fig. 1).

An ethanolic 2,6-diethylaniline solution (5 mmol, in 5 mL) was added to an aqueous HCl solution (0.5 M, 10 mL) at room temperature. Stable single crystals of 2,6-diethylphenylammonium chloride, with suitable dimensions, grew after some days of evaporation. The crystal structure of the title compound was determined using a single crystal. The experimental conditions of data collection, strategy used for the structure determination and the final results are given in Table 1. The structure was solved by direct methods and refined by full-matrix least-square based on \(F^2\) for all data with SHELXL97 software. All non-hydrogen atoms of \([2,6-(C_6H_5)C_6H_3NH_3]Cl\) were refined. The final atomic coordinates of the non-hydrogen atoms and their equivalent isotropic displacement parameters, \(U_{eq}\) are given in Table 2. The asymmetric unit of the title compound (Fig. 2) is composed of two 2,6-diethylphenylammonium cations and two chloride anions. A crystal-structure analysis showed the occurrence of hydrogen-bonding interactions between the anions and the cations associated with electrostatic and van der Walls interactions. In fact, the structure exhibits two types of hydrogen bonds (Table 3). The first one, N–H–Cl, with H–Cl distances ranging from 2.15 to 2.44 \(\text{Å}\), connects the ammonium cations and chloride anions to develop corrugated ribbons along the direction, while the pertinent angles fall in the interval of 144° to 167°. A platon analysis\(^4\) of (1) indicated the presence of a second type of C–H–Cl contacts that help to define the crystal packing in the title compound (Fig. 3). A structural comparison with related structures shows that these two kinds of hydrogen bonding, N–H–Cl as well as C–H–Cl, are very often encountered in the structure of these chloride salts and play an important role in building infinite networks with various geometries, such us ribbons, chains, layers and so on.\(^5\)

Two independent 2,6-diethylphenylammonium groups coexist

Table 1 Crystal and experimental data

<table>
<thead>
<tr>
<th>Chemical Formula: C(<em>{18})H(</em>{28})NCl</th>
<th>Formula weight: 185.69</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal system: monoclinic</td>
<td>(Z = 8)</td>
</tr>
<tr>
<td>Space group: (P2_1/a)</td>
<td>(a = 8.633(2), \text{Å})</td>
</tr>
<tr>
<td>(b = 20.530(2), \text{Å})</td>
<td>(\beta = 90.48(2)^\circ)</td>
</tr>
<tr>
<td>(c = 12.129(2), \text{Å})</td>
<td>(V = 2149.4(6), \text{Å}^3)</td>
</tr>
<tr>
<td>Linear absorption factor: (F(000) = 800)</td>
<td>(D_r = 1.148, \text{g cm}^{-3})</td>
</tr>
<tr>
<td>Crystal dimensions [mm]: 0.60 \times 0.30 \times 0.15</td>
<td>3.06 cm(^-3)</td>
</tr>
<tr>
<td>No. of reflections measured: 5146 ((R_{int} = 0.01))</td>
<td>2442 with (I &gt; 2\sigma(I))</td>
</tr>
<tr>
<td>No. of reflections used: 223</td>
<td>(R = 0.0565)</td>
</tr>
<tr>
<td>No. of parameters: 126 (Rcell)</td>
<td>(R_c = 0.1045)</td>
</tr>
<tr>
<td>Goodness-of-fit = 0.968</td>
<td>((\Delta \rho)_{max} = 0.211) e \text{ Å}^{-3})</td>
</tr>
<tr>
<td>((\Delta \rho)_{min} = -0.196) e \text{ Å}^{-3})</td>
<td>Measurement: Enraf-Nonius MACH3</td>
</tr>
<tr>
<td>Mo (K_a) (= 0.7107, \text{Å})</td>
<td>Program system: SHELXL 97</td>
</tr>
<tr>
<td>Structure determination: direct method</td>
<td>Refinement: full-matrix on (F^2)</td>
</tr>
<tr>
<td>Crystallographic Data Centre via <a href="http://www.ccdc.cam.ac.uk/data_request/cif">www.ccdc.cam.ac.uk/data_request/cif</a>.</td>
<td></td>
</tr>
</tbody>
</table>

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Fig. 1 Chemical diagram of the title compound.
Table 2 Final atomic coordinates and $U_{eq}$(Å$^2$) for the non hydrogen in [2,6-(C$_8$H$_5$)$_2$C$_6$H$_3$NH$_3^+$]Cl

<table>
<thead>
<tr>
<th>Atom</th>
<th>$x(\sigma)$</th>
<th>$y(\sigma)$</th>
<th>$z(\sigma)$</th>
<th>$U_{eq}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C11</td>
<td>0.73536(7)</td>
<td>0.22359(3)</td>
<td>0.73516(6)</td>
<td>0.04335(19)</td>
</tr>
<tr>
<td>C12</td>
<td>0.24665(10)</td>
<td>0.06703(3)</td>
<td>0.76291(7)</td>
<td>0.07218(3)</td>
</tr>
<tr>
<td>N1</td>
<td>1.0287(2)</td>
<td>0.17199(9)</td>
<td>0.72609(17)</td>
<td>0.04008(5)</td>
</tr>
<tr>
<td>N2</td>
<td>0.4331(2)</td>
<td>0.16070(9)</td>
<td>0.65226(17)</td>
<td>0.0405(5)</td>
</tr>
<tr>
<td>C1</td>
<td>0.9816(3)</td>
<td>0.15806(12)</td>
<td>-0.0263(2)</td>
<td>0.0377(6)</td>
</tr>
<tr>
<td>C2</td>
<td>0.896(3)</td>
<td>0.10179(12)</td>
<td>-0.0665(2)</td>
<td>0.0446(7)</td>
</tr>
<tr>
<td>C3</td>
<td>0.8604(3)</td>
<td>0.08979(15)</td>
<td>0.1039(3)</td>
<td>0.0594(8)</td>
</tr>
<tr>
<td>C4</td>
<td>0.800(4)</td>
<td>0.13215(18)</td>
<td>0.1835(3)</td>
<td>0.0676(9)</td>
</tr>
<tr>
<td>C5</td>
<td>0.9759(3)</td>
<td>0.18938(16)</td>
<td>0.1619(3)</td>
<td>0.0585(8)</td>
</tr>
<tr>
<td>C6</td>
<td>1.0177(3)</td>
<td>0.20474(13)</td>
<td>0.0553(2)</td>
<td>0.0441(7)</td>
</tr>
<tr>
<td>C7</td>
<td>1.0902(3)</td>
<td>0.26995(13)</td>
<td>0.0303(2)</td>
<td>0.0544(6)</td>
</tr>
<tr>
<td>C8</td>
<td>0.974(4)</td>
<td>0.31994(14)</td>
<td>-0.0122(3)</td>
<td>0.0714(10)</td>
</tr>
<tr>
<td>C9</td>
<td>0.8550(3)</td>
<td>0.05712(13)</td>
<td>-0.0996(3)</td>
<td>0.0621(9)</td>
</tr>
<tr>
<td>C10</td>
<td>0.742(2)</td>
<td>0.03319(17)</td>
<td>-0.0748(3)</td>
<td>0.0912(12)</td>
</tr>
<tr>
<td>C11</td>
<td>0.457(1)</td>
<td>0.13995(12)</td>
<td>0.5115(2)</td>
<td>0.0389(6)</td>
</tr>
<tr>
<td>C12</td>
<td>0.526(3)</td>
<td>0.16332(13)</td>
<td>0.4277(2)</td>
<td>0.0492(7)</td>
</tr>
<tr>
<td>C13</td>
<td>0.3906(4)</td>
<td>0.14187(16)</td>
<td>0.3227(3)</td>
<td>0.0671(9)</td>
</tr>
<tr>
<td>C14</td>
<td>0.5071(4)</td>
<td>0.09799(18)</td>
<td>0.3044(3)</td>
<td>0.0738(10)</td>
</tr>
<tr>
<td>C15</td>
<td>0.5974(4)</td>
<td>0.07463(15)</td>
<td>0.3857(3)</td>
<td>0.0623(9)</td>
</tr>
<tr>
<td>C16</td>
<td>0.5762(3)</td>
<td>0.09458(12)</td>
<td>0.4914(2)</td>
<td>0.0445(7)</td>
</tr>
<tr>
<td>C17</td>
<td>0.671(3)</td>
<td>0.06862(13)</td>
<td>0.5887(3)</td>
<td>0.0600(8)</td>
</tr>
<tr>
<td>C18</td>
<td>0.7146(4)</td>
<td>0.01902(16)</td>
<td>0.5607(3)</td>
<td>0.0887(12)</td>
</tr>
<tr>
<td>C19</td>
<td>0.2261(3)</td>
<td>0.20783(14)</td>
<td>0.4920(3)</td>
<td>0.0602(8)</td>
</tr>
<tr>
<td>C20</td>
<td>0.0851(3)</td>
<td>0.17022(16)</td>
<td>0.4880(3)</td>
<td>0.0805(11)</td>
</tr>
</tbody>
</table>

Estimated standard deviations are given in parentheses.

Table 3 Hydrogen bond scheme in [2,6-(C$_8$H$_5$)$_2$C$_6$H$_3$NH$_3^+$]Cl structure

<table>
<thead>
<tr>
<th>D-H...A</th>
<th>D-H(Å)</th>
<th>H...A(Å)</th>
<th>D...A(Å)</th>
<th>D-H...A(°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1-H1A..C31</td>
<td>0.89</td>
<td>2.43</td>
<td>3.194(2)</td>
<td>144</td>
</tr>
<tr>
<td>N1-H9B..C31</td>
<td>0.89</td>
<td>2.27</td>
<td>3.131(2)</td>
<td>164</td>
</tr>
<tr>
<td>N1-H1C..C12</td>
<td>0.89</td>
<td>2.21</td>
<td>3.087(2)</td>
<td>167</td>
</tr>
<tr>
<td>N2-H7A..C31</td>
<td>0.89</td>
<td>2.44</td>
<td>3.221(2)</td>
<td>147</td>
</tr>
<tr>
<td>N2-H2B..C11</td>
<td>0.89</td>
<td>2.32</td>
<td>3.193(2)</td>
<td>167</td>
</tr>
<tr>
<td>N2-H2C..C12</td>
<td>0.89</td>
<td>2.15</td>
<td>3.030(2)</td>
<td>167</td>
</tr>
<tr>
<td>C17-H1T..C31</td>
<td>0.97</td>
<td>2.78</td>
<td>3.682(3)</td>
<td>156</td>
</tr>
</tbody>
</table>

Fig. 2 ORTEP view of [2,6-(C$_8$H$_5$)$_2$C$_6$H$_3$NH$_3^+$]Cl. Thermal ellipsoid are given at 50% probability.

in this structure. The ethyl constituent conformations in the two independent ethylaminium are characterized by torsion angles of $10.5(4)^\circ$ and $79.3(3)^\circ$ for the first (A1) and $-0.1(4)^\circ$ and $-79.4(3)^\circ$ for the second (A2). Consequently, in each molecule, one ethyl group is flat and the other is perpendicular. These features are common in other structures containing this organic cation.5

References