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**Key indicators**

 Single-crystal X-ray study  
 $T = 120$  K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.054  
 $wR$  factor = 0.149  
 Data-to-parameter ratio = 18.6

 For details of how these key indicators were  
 automatically derived from the article, see  
<http://journals.iucr.org/e>.

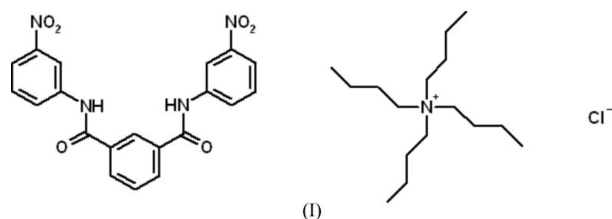
# *N,N'*-Bis(3-nitrophenyl)isophthalamide tetrabutylammonium chloride

 The receptor of the title compound,  $\text{C}_{14}\text{H}_{36}\text{N}^+\cdot\text{Cl}^- \cdot \text{C}_{20}\text{H}_{14}\text{N}_4\text{O}_6$ , binds a chloride anion *via* two  $\text{N}-\text{H}\cdots\text{Cl}$  hydrogen bonds [ $\text{N}\cdots\text{Cl} = 3.2367$  (14) Å and  $3.3239$  (15)°].

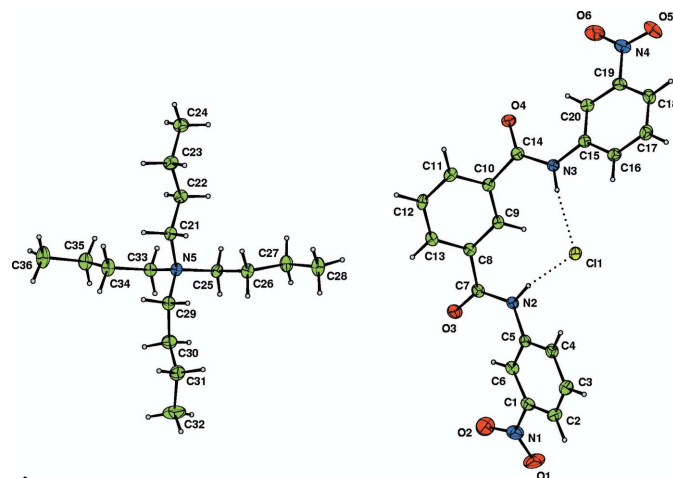
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**Comment**

This work forms part of an ongoing study on the conformational properties of the anion complexes of isophthalamides and their derivatives.



The receptor in the title chloride complex, (I), adopts a similar conformation to that of a bromide–isophthalamide complex reported by Kavallieratos *et al.* (1997). In both cases, the anion lies above the least-squares plane through the central aromatic ring. In the case of the chloride complex, the angle between the plane through the central aromatic ring and a plane defined by the anion and the amide H atoms is  $45.54$  (4)°, whilst for the larger bromide anion the angle was found to be  $63.63$  (6)°. The larger size of the bromide anion is also evident in the hydrogen-bond donor–acceptor distances, which were found to be  $3.634$  (4) and  $3.436$  (4) Å for the two  $\text{H}\cdots\text{Br}$  interactions, and are  $3.3239$  (15) and  $3.2367$  (14) Å for the  $\text{H}\cdots\text{Cl}$  interactions in the structure reported here (Table 1).


**Figure 1**

View of the asymmetric unit of (I), showing the atom labelling and the hydrogen-bonded chloride anion. Displacement ellipsoids are drawn at the 50% probability level and hydrogen bonds are shown as dashed lines.

It is interesting to note that the current chloride structure and the previous bromide structure form discrete 1:1 receptor–anion units, whilst the fluoride complex of a similar compound reported by Coles *et al.* (2003) forms a double helix with a 2:2 receptor-to-anion stoichiometry. This double unit is also present in the fluoride complex of a 1,3-diamido-anthraquinone (a ‘twisted’ isophthalamide analogue) reported by Brooks *et al.* (2005)

### Experimental

The title compound was prepared as reported previously by Moore *et al.* (1997) and Coles *et al.* (2003). Crystals were obtained by slow evaporation of a solution of the receptor in the presence of excess tetrabutylammonium chloride.

#### Crystal data

$C_{16}H_{36}N^+ \cdot Cl^- \cdot C_{20}H_{14}N_4O_6$   
 $M_r = 684.26$   
 Monoclinic,  $P2_1/n$   
 $a = 11.6508$  (2) Å  
 $b = 26.0390$  (4) Å  
 $c = 12.0569$  (2) Å  
 $\beta = 96.753$  (1)°  
 $V = 3632.39$  (10) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.251$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 24972 reflections  
 $\theta = 2.9$ – $27.5^\circ$   
 $\mu = 0.16$  mm<sup>-1</sup>  
 $T = 120$  (2) K  
 Slab, colourless  
 $0.60 \times 0.60 \times 0.10$  mm

#### Data collection

Bruker–Nonius KappaCCD diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SORTAV; Blessing, 1995)  
 $T_{\min} = 0.902$ ,  $T_{\max} = 0.985$   
 20923 measured reflections

8136 independent reflections  
 6851 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.078$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -15 \rightarrow 14$   
 $k = -31 \rightarrow 33$   
 $l = -14 \rightarrow 15$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.149$   
 $S = 0.99$   
 8136 reflections  
 438 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 1.9526P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.004$   
 $\Delta\rho_{\text{max}} = 0.43$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>  
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.0057 (16)

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2–H2A $\cdots$ Cl1	0.88	2.38	3.2367 (14)	163
N3–H3A $\cdots$ Cl1	0.88	2.46	3.3239 (15)	166

All H atoms were positioned with ideal geometry and allowed to ride on their parent atoms, with C–H = 0.95 (aromatic), 0.96 (methylene), 0.98 (methyl) and 0.88 Å (N–H), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic, methylene and NH H atoms})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: WinGX (Farrugia, 1999).

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