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N,*N*′,*N*″-Triphenylguanidinium bromide

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In the title compound, $C_{19}H_{18}N_3^+\cdot Br^-$, the dihedral angles between the phenyl ring planes and the plane defined by the central guanidinium fragment are in the range 43.1 (1)–64.0 (1)°. Intermolecular N—H···Br hydrogen bonds link the anions and cations into chains.

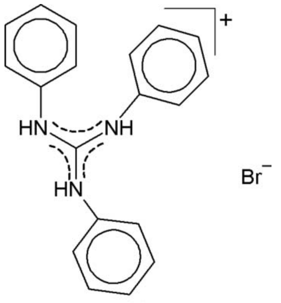
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.094
Data-to-parameter ratio = 19.4

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

Comment

Much of the interest in guanidine compounds and their derivatives is due to their biological activity, in particular their neuroleptic and antipsychotic properties (Weber *et al.*, 1986; Largent *et al.*, 1987). Our interest is focused on the physical properties of guanidine compounds, which are regarded as potentially interesting for applications in non-linear optics (Zyss *et al.*, 1993). We are currently investigating the structural, dielectric and optical properties of triphenylguanidine compounds.



(I)

In the title compound, (I), the central guanidine fragment of the cation is planar (Fig. 1), with bond lengths and angles close to those expected for a cental Csp^2 atom, accounting for some charge delocalization between the three C—N bonds. The bond lengths C1—N1 [1.330 (3) Å], C1—N2 [1.328 (3) Å] and C1—N3 [1.336 (3) Å] are comparable with literature averages for substituted and unsubstituted guanidinium cations (1.321 and 1.328 Å, respectively; Allen *et al.*, 1987). The dihedral angles between the phenyl ring planes and the plane defined by the central guanidinium fragment are 43.1 (1) (C2–C7), 63.4 (1) (C8–C13) and 64.0 (1)° (C14–C19). The corresponding angles for other reported triphenylguanidinium salts lie in the range 32.6 (3)–70.2 (3)° (Kemme *et al.*, 1988; Klement *et al.*, 1995; Pereira Silva *et al.*, 2006, 2007). The variability of these values shows the flexibility of the triphenylguanidinium cation.

The anions and cations in (I) are linked by N—H···Br hydrogen bonds into infinite chains running parallel to the c axis (Fig. 2 and Table 1).

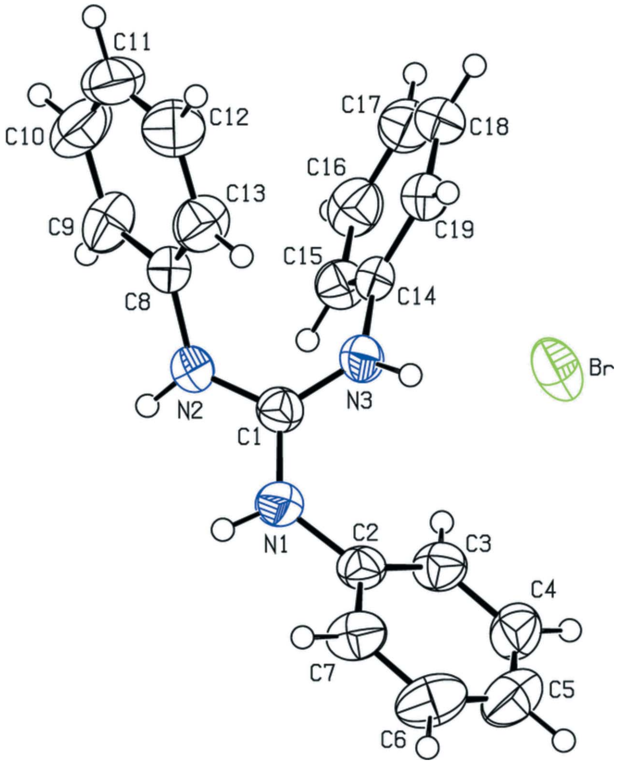


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms.

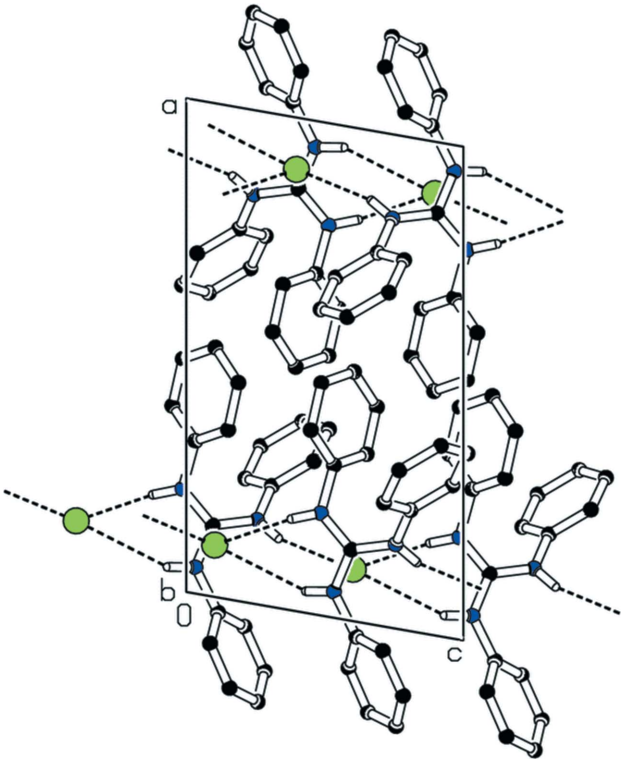


Figure 2
The packing in (I), viewed down the *b* axis, showing chains running along *c*. Dashed lines denote N—H···Br hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

Experimental

Hydrobromic acid (Aldrich, 48%, 0.06 mmol) was added to triphenylguanidine (Aldrich, 0.06 mmol) in a water–ethanol (1:1) solution (50 ml). The solution was warmed slowly and then left to evaporate under ambient conditions. Small transparent yellow crystals were deposited after a few days.

Crystal data

$C_{19}H_{18}N_3^+\cdot Br^-$
$M_r = 368.27$
Monoclinic, $P2_1/c$
$a = 13.9129$ (19) Å
$b = 16.195$ (5) Å
$c = 7.902$ (3) Å
$\beta = 100.10$ (2)°
$V = 1752.8$ (9) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 2.35$ mm^{-1}
$T = 293$ (2) K
0.30 × 0.26 × 0.16 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.539$, $T_{\max} = 0.687$
7432 measured reflections
4040 independent reflections
2716 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
3 standard reflections
frequency: 180 min
intensity decay: 9.5%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.094$
$S = 1.01$
4040 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.32$ e Å^{-3}
$\Delta\rho_{\min} = -0.48$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br^{i}	0.86	2.88	3.626 (3)	146
N2—H2···Br^{i}	0.86	2.45	3.212 (2)	147
N3—H3*A*···Br	0.86	2.44	3.270 (2)	163

Symmetry code: (i) $x, y, z + 1$.

H atoms were placed at calculated positions and refined as riding, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(C,N).

Data collection: CAD-4 (Enraf–Nonius, 1989); cell refinement: CAD-4; data reduction: *SDP*-Plus (Frenz, 1985); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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