The torsion angles most clearly illustrate the absence of an intramolecular mirror plane.

The observed value of the distance between the atoms C(1) and C(8) is 3·396 Å. The EFF calculated value is 3·525 Å. When the C(1)···C(8) distance and the valency angle at C(9) are constrained to the observed values during the EFF calculation, the energy rises 1·4 kJ mol^{-1} and m shows up again. An alternate empirical force field (EAS, Engler, Andose & von R. Schleyer, 1973) gives 3·602 Å for the non-bonded distance C(1)···C(8), 117·4° for the valency angle at C(9) and the energy increases by 3·3 kJ mol^{-1} when the observed values are used. Therefore, the prediction of geometric details of the strained structure of (I) using MM2 is better than with EAS. However, the former set of force-field parameters is also capable of improvement.

The crystals were provided by Dr D. Tavernier, State University at Gent, Belgium.

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Dimeric *tert*-Butylaminoboron Difluoride, $[(CH_3)_3CNHBF_2]_2$

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Abstract. $M_r = 241{\cdot}88$, orthorhombic, space group *Pbca*, $a = 7{\cdot}615\,(4)$, $b = 17{\cdot}007\,(8)$, $c = 9{\cdot}706\,(5)$ Å, $V = 1257\,(1)$ Å^3, $Z = 4$ (dimers), $D_x = 1{\cdot}278\,(1)$ g cm^{-3}, $F(000) = 512$, room temperature, $\lambda(\mathrm{Mo}\ K\alpha) = 0{\cdot}71069$ Å, $\mu(\mathrm{Mo}\ K\alpha) = 1{\cdot}1$ cm^{-1}, $R = 0{\cdot}037$ for 776 unique observed reflections. The dimers possess crystallographic inversion symmetry, with B—N 1·595 (4) Å, and B—F 1·355 (4) and 1·366 (4) Å. The B_2N_2 rings are exactly planar.

Introduction. The dehydrohalogenation of the title compound (1) (Elter, Glemser & Herzog, 1971; Greenwood, Hooton & Walker, 1966; Greenwood & Robinson, 1968) leads to (amongst other, non-cyclic, products) the tetrameric azaborane $[(CH_3)_3CNBF]_4$ (Elter, Noltemeyer & Sheldrick, 1984). We were therefore interested to discover whether (1) already contained the eight-membered BN ring in the solid state, or if, similarly to compounds R_2NBX_2 [R = Me, X = F, Hazell (1966); R = Et, X = F, Edwards & Stadler (1970); R = Me, X = Cl, Hess (1963)], it was dimeric. The molecular weight in solution suggests a dimeric formulation, although a tetramer gradually forms on standing (Greenwood *et al.*, 1966).

Experimental. D_m not determined. Colourless rhombic prisms, sealed in glass capillaries to prevent slow hydrolysis by atmospheric moisture. Stoe two-circle diffractometer, monochromated Mo $K\alpha$ radiation. Crystal 1, mounted about **c**, 0·45 × 0·4 × 0·2 mm, layers 0–7, 1029 reflections. Crystal 2, mounted about **a**, 0·55 × 0·45 × 0·3 mm, layers 0–7, 1495 reflections. Interlayer scale factors derived from least-squares analysis of common reflections after Lp corrections. No absorption correction. 870 unique reflections (R_{int} 0·023, $2\theta_{\max}$ 55°), of which 776 with $F > 4\sigma(F)$ used for all calculations. Cell constants refined from ω values of 231 strong reflections from various positive and negative layers (Clegg & Sheldrick, 1984). Structure solution by routine direct methods. Refinement on F to R 0·037, R_w 0·036 [non-H atoms anisotropic, H(1) refining freely isotropic, other H using riding model

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with C—H 0·96 Å, H—C—H 109·5°, $U(\mathrm{H}) = 1{\cdot}2\,U_{\mathrm{eq}}(\mathrm{C})$; weighting scheme $w^{-1} = \sigma^2(F) + 0{\cdot}0001F^2$; 86 parameters, $S = 2{\cdot}0$, slope of normal probability plot 1·6]. Max. Δ/σ 0·002; max. and min. heights in final $\Delta\rho$ map +0·16, −0·14 e Å^{-3}. No correction for secondary extinction. Calculations performed with program system *SHELXTL* (Sheldrick, 1978).

Discussion. Final atomic coordinates and derived parameters are given in Tables 1 and 2.* The structure is shown in Figs. 1 and 2. Compound (1) is dimeric; since the dimers possess a crystallographic centre of symmetry, the B_2N_2 ring is constrained to be exactly planar. The B—N and B—F bond lengths are similar to those of the other R_2NBX_2 dimers, although the low accuracy of the earlier studies precludes useful comparisons. The shortest intermolecular contacts between non-H atoms are F(2)···C(2) 3·18 (2), F(1)···N(1) 3·29 (2) Å (second atoms at $-1+x,y,z$; $-0{\cdot}5+x,y,1{\cdot}5-z$ respectively).

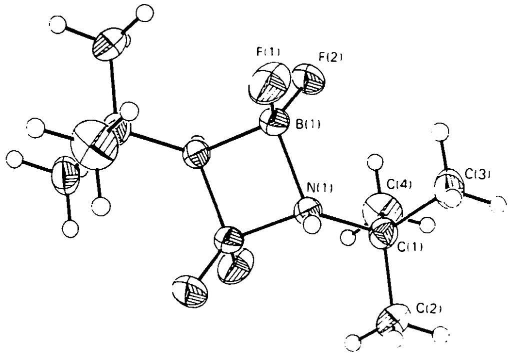

Fig. 1. Thermal-ellipsoid plot (50% level) of (1) showing the numbering scheme.

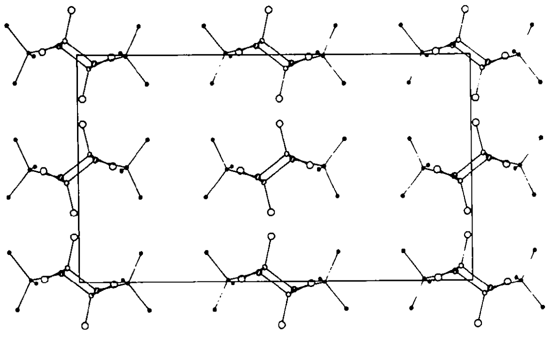

Fig. 2. Packing plot of (1) projected down **a**.

Table 1. *Atom coordinates* (×10^4) *and isotropic temperature factors* (Å^2 ×10^3)

	x	y	z	U_{eq} or U_{iso}
C(1)	6827 (2)	1234 (1)	5062 (2)	42 (1)†
C(2)	8790 (2)	1105 (1)	4923 (2)	59 (1)†
H(21)	9392	1591	4755	71
H(22)	8985	754	4163	71
H(23)	9230	871	5755	71
C(3)	6435 (3)	1772 (1)	6273 (2)	59 (1)†
H(31)	7002	2267	6110	71
H(32)	6854	1552	7123	71
H(33)	5188	1850	6329	71
C(4)	6089 (3)	1582 (1)	3739 (2)	74 (1)†
H(41)	6357	1254	2962	89
H(42)	6605	2092	3608	89
H(43)	4838	1635	3824	89
N(1)	6009 (2)	445 (1)	5384 (2)	37 (1)†
H(1)	6488 (21)	310 (9)	6099 (17)	25 (5)
B(1)	3959 (3)	300 (1)	5613 (3)	52 (1)†
F(1)	3589 (2)	123 (1)	6954 (1)	83 (1)†
F(2)	2925 (2)	882 (1)	5110 (2)	84 (1)†

† $U_{\mathrm{eq}} = \frac{1}{3}\sum_i\sum_j U_{ij}a^*_i a^*_j \mathbf{a}_i.\mathbf{a}_j$.

Table 2. *Bond lengths* (Å) *and angles* (°)

C(1)—C(2)	1·517 (4)	C(1)—C(3)	1·519 (4)
C(1)—C(4)	1·522 (4)	C(1)—N(1)	1·512 (3)
B(1)—N(1)	1·595 (4)	B(1)—F(1)	1·366 (4)
B(1)—F(2)	1·355 (4)	N(1)—H(1)	0·82 (2)
C(2)—C(1)—C(3)	110·5 (3)	C(2)—C(1)—C(4)	110·2 (3)
C(3)—C(1)—C(4)	110·2 (3)	C(2)—C(1)—N(1)	107·3 (2)
C(3)—C(1)—N(1)	107·1 (2)	C(4)—C(1)—N(1)	111·6 (3)
C(1)—N(1)—B(1)	124·7 (2)	C(1)—N(1)—B(1^{i})	125·0 (3)
B(1)—N(1)—B(1^{i})	88·7 (2)	N(1)—B(1)—F(1)	111·6 (3)
N(1)—B(1)—F(2)	114·0 (3)	F(1)—B(1)—F(2)	112·6 (3)
N(1)—B(1)—N(1^{i})	91·3 (2)	F(1)—B(1)—N(1^{i})	114·0 (3)
F(2)—B(1)—N(1^{i})	111·7 (3)		

Symmetry operator: (i) $1-x, -y, 1-z$.

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