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1,4-Bis(2,4,6-trimethylphenyl)-1,4-diazabuta-1,3-diene

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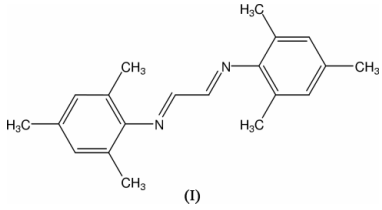
The title compound, $C_{20}H_{24}N_2$, (I), has crystallographic C_i symmetry, with the central C—C bond located on a centre of inversion. The dihedral angle between the central 1,4-diaza-buta-1,3-diene moiety and the attached substituted phenyl ring is 64.0 (2) Å.



(I)

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.047
wR factor = 0.125
Data-to-parameter ratio = 15.4

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

Experimental

The title compound, (I), was prepared during our studies on stabilized silylium ions by reaction of glyoxal with two molar equivalents of 2,4,6-trimethylaniline in aqueous methanol, in the presence of catalytic amounts of glacial acetic acid at 273 K (Tom Diek *et al.*, 1981). Recrystallization from THF gave orange–yellow crystals suitable for X-ray analysis.

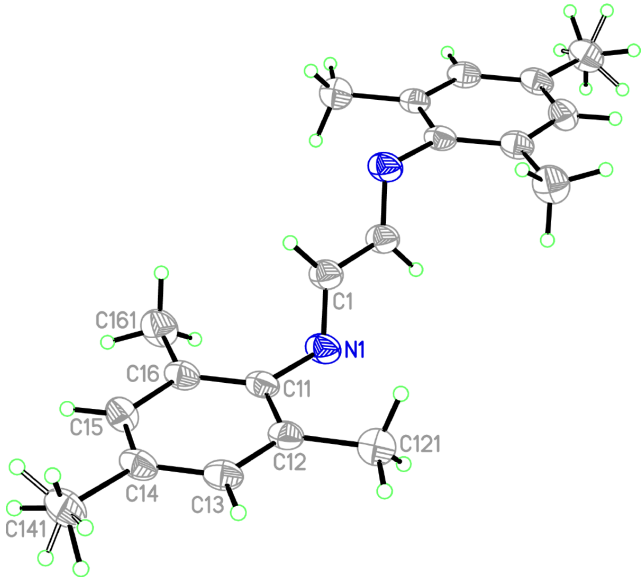


Figure 1
A perspective view of the title compound with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level. Only the symmetry-independent atoms are labelled. The unlabelled part is related by the symmetry code $(-x, 1-y, 1-z)$.

Crystal data

$C_{20}H_{24}N_2$	D_x = 1.118 Mg m^{-3}
M_r = 292.41	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4522 reflections
a = 13.486 (1) Å	θ = 1–25°
b = 4.403 (1) Å	μ = 0.07 mm^{-1}
c = 15.435 (1) Å	T = 173 K
β = 108.65 (1)°	Block, orange–yellow
V = 868.4 (2) Å^3	0.32 × 0.30 × 0.28 mm
Z = 2	

Data collection

Siemens CCD three-circle diffractometer	1167 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.044
Absorption correction: none	θ_{max} = 25.4°
11184 measured reflections	$h = -16 \rightarrow 16$
1597 independent reflections	$k = -5 \rightarrow 5$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.332P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.125	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
1597 reflections	
104 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.273 (2)	C1—C1^{i}	1.463 (3)
N1—C11	1.436 (2)		
C1—N1—C11	117.88 (15)	N1—C1—C1^{i}	120.1 (2)

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

All H atoms were located by difference Fourier synthesis and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5 U_{eq}(C_{methyl})], using a riding model with aromatic C—H = 0.95 Å and methyl C—H = 0.98 Å. The methyl groups were allowed to rotate about their local threefold axes. The H atoms at C14 are disordered over two orientations rotated from each other by 60°. The ratio of their site-occupation factors refined to 0.64 (2)/0.36 (2).

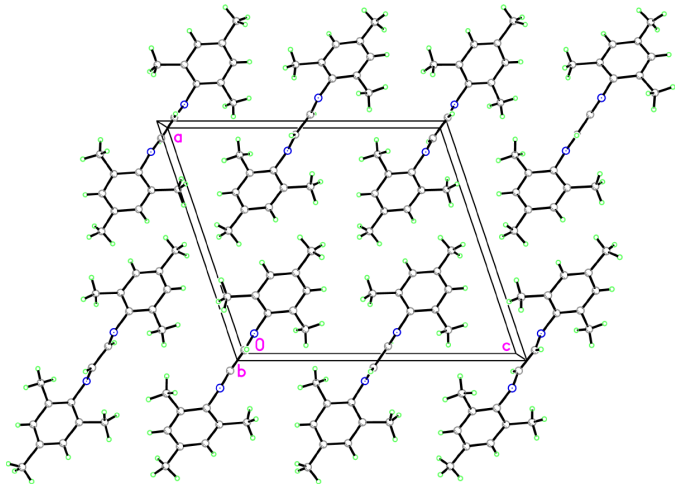


Figure 2
Packing diagram of the title compound, viewed along the *b* axis.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *PLATON* (Spek, 1990).

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