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

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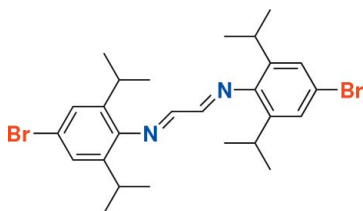
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Key indicators: single-crystal X-ray study; $T = 300$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.069; wR factor = 0.199; data-to-parameter ratio = 16.1.

The molecule of the title compound, $\text{C}_{26}\text{H}_{34}\text{Br}_2\text{N}_2$, lies on a crystallographic inversion center and hence the two imine groups are *s-trans*. The dihedral angle between the central 1,4-diazabuta-1,3-diene unit and the attached substituted phenyl ring is $88.4(7)^\circ$. The structure features a $\text{C}-\text{H}\cdots\text{N}$ close contact. The crystal selected for this study proved to be a non-merohedral twin with a minor component of 21.8 (3)%.

Related literature

1,4-diaza-1,3-butadiene (DAB) ligands containing sterically demanding *N*-substituents have proved to be versatile platforms for stabilizing *s*- and *p*-block atoms in unusual oxidation states or coordination geometries, see: Baker et al. (2008); Hill et al. (2009); Liu et al. (2009); Martin et al. (2009); Segawa et al. (2008). The title compound was prepared as part of our continuing studies on the chemistry of *N*-heterocyclic silylenes and germynes, see: Hill et al. (2005); Naka et al. (2004); Tomasik et al. (2009). For the use of DAB ligands in olefin polymerization catalysis, see: Ittel et al. (2000); Jung et al. (2007). For related structures, see: (2003); Müller et al. (2003); Schaub et al. (2006); Berger et al. (2001); Laine et al. (1999). For the preparation of 4-bromo-2,6-di-iso-propyl aniline, see: Liu et al. (2005). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$\text{C}_{26}\text{H}_{34}\text{Br}_2\text{N}_2$
 $M_r = 534.37$
 Monoclinic, $P2_1/c$
 $a = 8.961(3)$ Å
 $b = 17.848(7)$ Å
 $c = 8.620(3)$ Å
 $\beta = 104.260(11)^\circ$
 $V = 1336.2(8)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 3.05$ mm⁻¹
 $T = 300$ K
 $0.43 \times 0.35 \times 0.29$ mm

Data collection

Bruker SMART X2S diffractometer
 Absorption correction: multi-scan (TWINABS; Bruker, 2007)
 $T_{\min} = 0.103$, $T_{\max} = 0.428$
 2286 measured reflections
 2286 independent reflections
 1585 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.110$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.069$
 $wR(F^2) = 0.199$
 $S = 1.04$
 2286 reflections
 142 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.53$ e Å⁻³
 $\Delta\rho_{\min} = -0.60$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C8}-\text{H8}\cdots\text{N1}$	0.98	2.40	2.880 (9)	109

Data collection: *GIS* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* and *OLEX2* (Dolomanov et al., 2009); molecular graphics: *SHELXTL* and *OLEX2*; software used to prepare material for publication: *SHELXTL*, *OLEX2* (Dolomanov et al., 2009), *publCIF* (Westrip, 2009) and *modiCIFer* (Guzei, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2248).

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supplementary materials

Acta Cryst. (2010). E66, o40-o41 [doi:10.1107/S1600536809050843]

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

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Comment

1,4-diaza-1,3-butadiene (DAB) ligands bearing bulky aryl or alkyl groups on the nitrogen atoms have proven to be versatile platforms for stabilizing *s*- and *p*-block atoms in unusual oxidation states or coordination geometries (Baker *et al.* (2008); Hill *et al.* (2009); Liu *et al.* (2009); Martin *et al.* (2009); Segawa *et al.* (2008)). The title compound, (I), was prepared as part of our continuing studies upon the chemistry of N-heterocyclic silylenes and germynes (Hill *et al.* (2005); Naka *et al.* (2004); Tomasik *et al.* (2009)), the silicon(II) and germanium(II) analogues of the well known Arduengo N-heterocyclic carbenes. DAB ligands are ideal in this regard since their stereo-electronic properties are easily tuned by alteration of the N- and C-substituents.

DAB ligands have also been used extensively in d-block coordination chemistry, particularly within the field of olefin polymerization catalysis (Ittel *et al.* 2000). Jung *et al.* (2007) recently used the title compound as a precursor to an N-heterocyclic carbene in the synthesis of a catalytically active cationic (η^3 -allyl)(NHC)palladium complex.

The molecule of (I) resides on a crystallographic inversion center and hence the two imine groups are *s-trans*. The dihedral angle between the central 1,4-diazabuta-1,3-diene moiety and the attached substituted phenyl ring is 88.4 (7)°. The molecular symmetry approaches C_{2h}, however, the positions of the isopropyl groups break the mirror plane symmetry: both H atoms on the tertiary C atoms of the two symmetry-independent ⁱPr groups point toward atom N1, but reside on the opposite sides of the phenyl ring. This is illustrated with two disparate but "would be equivalent" torsion angles, one for each ⁱPr group: C2—C3—C8—C9 (-96.5 (8)°) and C2—C7—C11—C13 (163.6 (7)°). This geometry differs from that of the unbrominated congener of (I), 1,4-bis(2,6-diisopropyl-phenyl)-1,4-diazabuta-1,3-diene, (II). For related structures, see: Müller *et al.* (2003), Schaub *et al.* (2006). Compound (II), structurally characterized at 173 K by Berger *et al.* (2001) and at 193 K by Laine *et al.* (1999), crystallizes with the molecule of (II) on an inversion center. The H atoms of the tertiary C atom of the isopropyl groups point toward the N atom and, in contrast to (I), are located on the same side of the phenyl ring. The overall symmetry of (II) is much closer to C_{2h} as the ⁱPr groups are oriented very similarly: in the 193 K structure of (II) two "would be equivalent" Me—C(H)—C—C(N) torsion angles measured 144.6 and 145.4°. The C—Br distance of 1.897 (6) Å is in excellent agreement with the value of 1.899 (11) Å obtained by averaging 2303 C—Br bond lengths from 1736 relevant compounds reported to the Cambridge Structural Database (Allen, 2002).

Experimental

4-Bromo-2,6-di-*iso*-propyl aniline was prepared according to the literature procedure (Liu *et al.* 2005). To a stirred solution of 4-bromo-2,6-di-*iso*-propyl aniline (3.0 g, 11.71 mmol) in methanol (40 cm³) containing 4 drops of formic acid was added glyoxal (0.85 g, 5.80 mmol, 40% aqueous soln.) slowly dropwise. The reaction mixture was stirred for 24 h at room temperature, filtered, and the precipitate washed with cold MeOH (2 x 10 mL). This yellow solid was dried *in vacuo* and recrystallized from EtOH to give a crop of pale yellow needles suitable for X-ray diffraction analysis. Yield 3.53 g, 56%.

supplementary materials

$^1\text{H-NMR}$ (CD_2Cl_2 , 300 MHz): δ 1.19 (d, $^3J=6.9$ Hz, 24H, CH_3), 2.91 (sept, $^3J=6.8$ Hz, 4H, CH), 7.31 (s, 4H, aromatic), 8.07 (s, 2H, CH); $^{13}\text{C}\{^1\text{H}\}$ -NMR (CD_2Cl_2 , 75 MHz): δ 22.80, 28.43, 119.42, 126.79, 139.29, 147.52, 163.97.

Refinement

All H-atoms were placed in idealized locations with C—H distances 0.93 - 0.98 Å and refined as riding with appropriate thermal displacement coefficients $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times $U_{\text{eq}}(\text{bearing atom})$. The crystal of (I) selected for this study proved to be a non-merohedral twin. The two twin components are related by a 179.9° rotation about the [001] direction in reciprocal space with the minor component contribution of 21.8 (3)%.

Figures

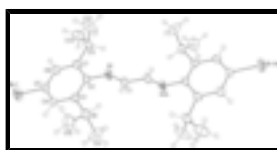


Fig. 1. Molecular structure of (I). The thermal ellipsoids are shown at 30% probability level. Atoms labeled with the suffixes A and unlabeled are generated by the symmetry operation $(-x+I, -y+I, -z+I)$.

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Crystal data

$\text{C}_{26}\text{H}_{34}\text{Br}_2\text{N}_2$

$M_r = 534.37$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.961$ (3) Å

$b = 17.848$ (7) Å

$c = 8.620$ (3) Å

$\beta = 104.260$ (11) $^\circ$

$V = 1336.2$ (8) Å³

$Z = 2$

$F(000) = 548$

$D_x = 1.328$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 999 reflections

$\theta = 2.3$ – 24.8°

$\mu = 3.05$ mm⁻¹

$T = 300$ K

Block, yellow

$0.43 \times 0.35 \times 0.29$ mm

Data collection

Bruker SMART X2S
diffractometer

Radiation source: micro-focus sealed tube
doubly curved silicon crystal

ω scans

Absorption correction: multi-scan
(TWINABS; Bruker, 2007)

$T_{\text{min}} = 0.103$, $T_{\text{max}} = 0.428$

2286 measured reflections

2286 independent reflections

1585 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.110$

$\theta_{\text{max}} = 24.8^\circ$, $\theta_{\text{min}} = 2.3^\circ$

$h = 0 \rightarrow 10$

$k = -21 \rightarrow 0$

$l = -10 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.069$	H-atom parameters constrained
$wR(F^2) = 0.199$	$w = 1/[\sigma^2(F_o^2) + (0.0949P)^2 + 1.843P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
2286 reflections	$(\Delta/\sigma)_{\max} = 0.001$
142 parameters	$\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXTL</i> (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001 \times Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.038 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	1.14981 (9)	0.69711 (6)	0.27272 (12)	0.0957 (6)
N1	0.6097 (6)	0.5812 (3)	0.5079 (7)	0.0523 (14)
C1	0.5657 (8)	0.5148 (3)	0.4744 (8)	0.0513 (17)
H1	0.6173	0.4847	0.4166	0.062*
C2	0.7381 (6)	0.6090 (3)	0.4544 (7)	0.0395 (14)
C3	0.7094 (7)	0.6469 (3)	0.3074 (7)	0.0409 (14)
C4	0.8336 (7)	0.6738 (3)	0.2564 (7)	0.0456 (15)
H4	0.8179	0.6992	0.1595	0.055*
C5	0.9804 (7)	0.6630 (4)	0.3489 (8)	0.0500 (16)
C6	1.0083 (7)	0.6289 (4)	0.4968 (8)	0.0529 (16)
H6	1.1086	0.6245	0.5591	0.063*
C7	0.8860 (8)	0.6012 (3)	0.5528 (8)	0.0485 (16)
C8	0.5477 (7)	0.6575 (4)	0.2044 (9)	0.0536 (16)
H8	0.4780	0.6500	0.2746	0.064*
C9	0.5079 (12)	0.5984 (6)	0.0770 (14)	0.119 (4)
H9C	0.5672	0.6062	-0.0004	0.179*

supplementary materials

H9B	0.4002	0.6013	0.0251	0.179*
H9A	0.5309	0.5498	0.1247	0.179*
C10	0.5185 (9)	0.7356 (5)	0.1375 (14)	0.088 (3)
H10C	0.5496	0.7714	0.2224	0.132*
H10A	0.4108	0.7416	0.0883	0.132*
H10B	0.5766	0.7436	0.0590	0.132*
C11	0.9157 (9)	0.5652 (4)	0.7203 (8)	0.0626 (18)
H11	0.8533	0.5195	0.7090	0.075*
C12	0.8601 (13)	0.6152 (5)	0.8316 (10)	0.101 (3)
H12B	0.8573	0.5880	0.9269	0.151*
H12A	0.7586	0.6327	0.7808	0.151*
H12C	0.9285	0.6572	0.8591	0.151*
C13	1.0834 (11)	0.5415 (5)	0.7895 (10)	0.087 (3)
H13A	1.1158	0.5093	0.7148	0.131*
H13B	1.0915	0.5152	0.8884	0.131*
H13C	1.1478	0.5852	0.8086	0.131*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0555 (5)	0.1428 (10)	0.0961 (8)	-0.0228 (5)	0.0324 (5)	0.0295 (6)
N1	0.067 (3)	0.034 (3)	0.065 (4)	-0.011 (2)	0.036 (3)	-0.001 (2)
C1	0.068 (4)	0.035 (3)	0.063 (4)	-0.014 (3)	0.040 (4)	-0.007 (3)
C2	0.053 (3)	0.027 (3)	0.046 (4)	-0.006 (2)	0.026 (3)	-0.004 (3)
C3	0.046 (3)	0.033 (3)	0.046 (4)	-0.005 (3)	0.015 (3)	-0.003 (3)
C4	0.053 (4)	0.046 (3)	0.039 (3)	-0.006 (3)	0.014 (3)	0.002 (3)
C5	0.046 (4)	0.059 (4)	0.050 (4)	-0.011 (3)	0.021 (3)	0.000 (3)
C6	0.052 (3)	0.057 (4)	0.050 (4)	-0.006 (3)	0.014 (3)	0.006 (3)
C7	0.064 (4)	0.042 (3)	0.043 (4)	-0.006 (3)	0.020 (3)	0.002 (3)
C8	0.046 (3)	0.052 (4)	0.063 (4)	-0.005 (3)	0.014 (3)	0.007 (3)
C9	0.093 (7)	0.119 (8)	0.117 (9)	-0.024 (6)	-0.030 (6)	-0.045 (7)
C10	0.063 (5)	0.080 (5)	0.115 (8)	0.008 (4)	0.013 (6)	0.039 (6)
C11	0.083 (5)	0.059 (4)	0.052 (4)	-0.003 (4)	0.027 (4)	0.014 (4)
C12	0.161 (10)	0.094 (6)	0.063 (6)	0.043 (6)	0.058 (6)	0.026 (5)
C13	0.109 (7)	0.081 (6)	0.072 (6)	0.025 (5)	0.025 (5)	0.019 (5)

Geometric parameters (\AA , $^\circ$)

Br1—C5	1.897 (6)	C8—H8	0.9800
N1—C1	1.260 (7)	C9—H9C	0.9600
N1—C2	1.429 (7)	C9—H9B	0.9600
C1—C1 ⁱ	1.455 (11)	C9—H9A	0.9600
C1—H1	0.9300	C10—H10C	0.9600
C2—C7	1.393 (9)	C10—H10A	0.9600
C2—C3	1.403 (8)	C10—H10B	0.9600
C3—C4	1.380 (8)	C11—C12	1.483 (11)
C3—C8	1.513 (9)	C11—C13	1.533 (12)
C4—C5	1.374 (9)	C11—H11	0.9800

C4—H4	0.9300	C12—H12B	0.9600
C5—C6	1.379 (9)	C12—H12A	0.9600
C6—C7	1.393 (9)	C12—H12C	0.9600
C6—H6	0.9300	C13—H13A	0.9600
C7—C11	1.542 (9)	C13—H13B	0.9600
C8—C9	1.501 (12)	C13—H13C	0.9600
C8—C10	1.507 (10)		
C1—N1—C2	118.9 (5)	C8—C9—H9B	109.5
N1—C1—C1 ⁱ	120.3 (7)	H9C—C9—H9B	109.5
N1—C1—H1	119.9	C8—C9—H9A	109.5
C1 ⁱ —C1—H1	119.9	H9C—C9—H9A	109.5
C7—C2—C3	122.3 (5)	H9B—C9—H9A	109.5
C7—C2—N1	119.3 (5)	C8—C10—H10C	109.5
C3—C2—N1	118.4 (5)	C8—C10—H10A	109.5
C4—C3—C2	118.2 (5)	H10C—C10—H10A	109.5
C4—C3—C8	120.0 (5)	C8—C10—H10B	109.5
C2—C3—C8	121.8 (5)	H10C—C10—H10B	109.5
C5—C4—C3	119.9 (6)	H10A—C10—H10B	109.5
C5—C4—H4	120.1	C12—C11—C13	111.5 (8)
C3—C4—H4	120.1	C12—C11—C7	110.3 (6)
C4—C5—C6	121.9 (6)	C13—C11—C7	114.0 (6)
C4—C5—Br1	119.2 (5)	C12—C11—H11	106.9
C6—C5—Br1	118.9 (5)	C13—C11—H11	106.9
C5—C6—C7	119.9 (6)	C7—C11—H11	106.9
C5—C6—H6	120.1	C11—C12—H12B	109.5
C7—C6—H6	120.1	C11—C12—H12A	109.5
C6—C7—C2	117.7 (6)	H12B—C12—H12A	109.5
C6—C7—C11	120.2 (6)	C11—C12—H12C	109.5
C2—C7—C11	122.1 (6)	H12B—C12—H12C	109.5
C9—C8—C10	112.5 (8)	H12A—C12—H12C	109.5
C9—C8—C3	111.2 (6)	C11—C13—H13A	109.5
C10—C8—C3	113.0 (5)	C11—C13—H13B	109.5
C9—C8—H8	106.5	H13A—C13—H13B	109.5
C10—C8—H8	106.5	C11—C13—H13C	109.5
C3—C8—H8	106.5	H13A—C13—H13C	109.5
C8—C9—H9C	109.5	H13B—C13—H13C	109.5
C2—N1—C1—C1 ⁱ	-179.3 (8)	C5—C6—C7—C11	-178.1 (6)
C1—N1—C2—C7	-90.5 (7)	C3—C2—C7—C6	-3.5 (9)
C1—N1—C2—C3	92.9 (7)	N1—C2—C7—C6	-179.9 (6)
C7—C2—C3—C4	3.3 (8)	C3—C2—C7—C11	174.9 (5)
N1—C2—C3—C4	179.8 (5)	N1—C2—C7—C11	-1.6 (8)
C7—C2—C3—C8	-177.7 (5)	C4—C3—C8—C9	82.5 (8)
N1—C2—C3—C8	-1.2 (8)	C2—C3—C8—C9	-96.4 (8)
C2—C3—C4—C5	0.1 (9)	C4—C3—C8—C10	-45.1 (9)
C8—C3—C4—C5	-178.9 (6)	C2—C3—C8—C10	135.9 (7)
C3—C4—C5—C6	-3.3 (10)	C6—C7—C11—C12	108.2 (9)
C3—C4—C5—Br1	177.6 (5)	C2—C7—C11—C12	-70.1 (9)
C4—C5—C6—C7	3.1 (10)	C6—C7—C11—C13	-18.1 (10)

supplementary materials

Br1—C5—C6—C7	-177.8 (5)	C2—C7—C11—C13	163.6 (7)
C5—C6—C7—C2	0.3 (9)		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C8—H8 \cdots N1	0.98	2.40	2.880 (9)	109

Fig. 1

