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2,3-Bis(2-*tert*-butylphenylimino)butane

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In the title compound, $C_{24}H_{32}N_2$, there is one half-molecule in the asymmetric unit, the other half being generated by inversion. All bond lengths and angles show normal values. The deviation from a planar arrangement can be attributed to non-classical hydrogen bonds and steric factors.

Comment

The study of new catalysts for olefin polymerization has grown considerably over the last few years. α-Diimines have been the preferred ligands for the synthesis of this class of catalysts (Brookhart's catalysts) (Rix & Brookhart, 1995). In addition to the metal, the choice of a suitable ligand can bring more satisfactory results, depending on the reaction under study. The type of substituents on the aromatic ring of the α-diimine has a direct influence on the degree of polymerization. The literature reports that neutral α-diimine nickel(II) complexes with bulky substituents lead to an effective polymerization of ethylene, yielding high molecular weight polymers (Wang *et al.*, 1998). On the other hand, cationic nickel(II) and palladium(II) complexes with the same ligands were capable of polymerizing olefins, *R*-olefins, and cyclic olefins to high molecular weight polymers (Johnson *et al.*, 1995). The present communication describes the chief characteristics of 2,3-bis(2-tertbutyl)iminobutane, (I) (Fig. 1).

(I)
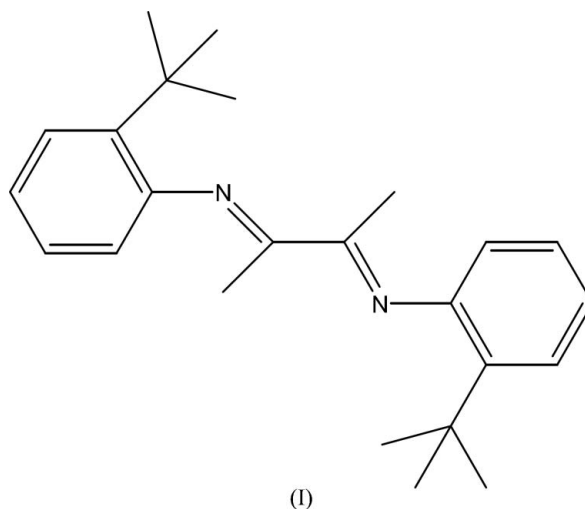
The centrosymmetric molecule under discussion can be described in terms of its intramolecular interactions and its steric factor, the latter being of enormous importance because of the bulky substituent on the aromatic ring. Two non-classical hydrogen bonds are observed, *viz*. C10—H10*A*···N1, and C12—H12*A*···N1. It is believed that the deviation
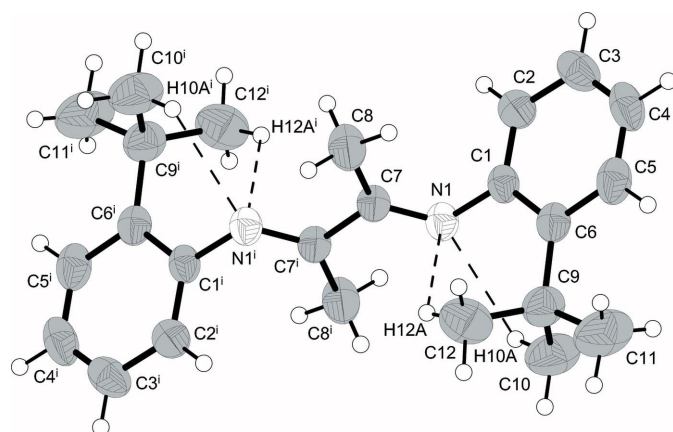
Figure 1
View of (I) (50% probability displacement ellipsoids). The dashed lines indicate the proposed non-classical intramolecular hydrogen bonds. [Symmetry code: (i) $1 - x$, $1 - y$, $-z$.]
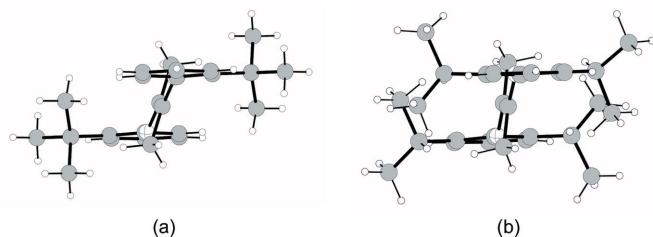

Figure 2
Comparison of the structures of (*a*) (I) and (*b*) 2,3-bis(2,6-diisopropyl)iminobutane.

between the planes formed by atoms C1–C2–C3–C4–C5–C6 and C8–C7–N1 is related to the presence of those interactions, as well as to the *tert*-butyl and methyl groups present in the molecule (Fig. 2*a*). The angle formed by the planes is 69.6 (1)°. The literature describes α-diimines with either bulky diisopropyl, *e.g.* 2,3-bis(2,6-diisopropyl)iminobutane (Cope-Eatough *et al.*, 2003) (Fig. 2*b*), or non-bulky methyl, *e.g.* 2,3-bis(2,6-dimethyl)iminobutane (Kuhn *et al.*, 2001), substituents on the 2 and 6 positions of the aromatic ring, which do not present a deviation as great as that of the present molecule. The fact that we only have a single substituent leads to the conformation obtained, insofar as there is only one possibility of interaction between the imine N atom and one of the H atoms present in the *tert*-butyl group.

The values found for the C—N distances (Table 1) agree well with what is expected for this bonding mode, as described in the literature (Allen *et al.*, 1987).

Experimental

2-*tert*-Butylaniline (2,086 g, 14 mmol) was added slowly at room temperature to a methanol solution (15 ml) of 2,3-butanedione (0.602 g, 7 mmol) in the presence of a catalytic amount of formic acid. After 2 h of magnetic stirring, the crude yellow product was isolated by filtration, washed with cold methanol (3 × 10 ml) and dried in a vacuum. Yellow block-shaped crystals suitable for X-ray diffraction were obtained by recrystallization from a dichloromethane solution (yield: 2.144 g, 88%; m.p. 383 K).

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.4185 (17)	C7—C8	1.496 (2)
C7—N1	1.2772 (17)	C7—C7^i	1.495 (3)
N1—C7—C8	126.45 (14)	C8—C7—C7^i	117.46 (16)
N1—C7—C7^i	116.03 (15)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C10—H10A$\cdots$N1	0.98 (2)	2.47 (2)	3.097 (3)	121.5 (15)
C12—H12A$\cdots$N1	1.02 (2)	2.41 (3)	3.065 (3)	121.7 (18)

All H atoms were located in a Fourier difference map and refined freely.

Data collection: *COSMO* and *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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