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(*E,E*)-*N*-[3-(Biphenyl-2-ylimino)butan-2-ylidene]-2-phenylaniline

 Hao Zou,^a Yubang Hou,^b Xuejian Yong,^b Yunbin Cen^b and Feng Bao^{b*}
^aInstitute of Polymer Science, School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Guangzhou 510275, People's Republic of China, and ^bDepartment of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

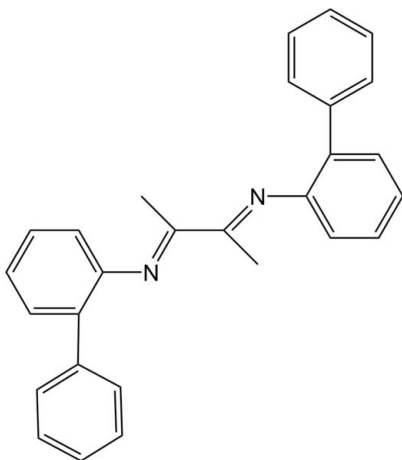
Correspondence e-mail: baofengstorm@126.com

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 Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.049; wR factor = 0.178; data-to-parameter ratio = 17.3.

The two $\text{C}=\text{N}$ double bonds in the structure of the title compound, $\text{C}_{28}\text{H}_{24}\text{N}_2$, lie in the same plane with a bond length of 1.269 (2) Å. The molecule is positioned on a centre of symmetry.

Related literature

 For related literature, see: Bao *et al.* (2005); Bao, Lü *et al.* (2006); Bao, Ma *et al.* (2006); Zou *et al.* (2005).


Experimental

Crystal data

 $\text{C}_{28}\text{H}_{24}\text{N}_2$
 $M_r = 388.49$
 Monoclinic, $P2_1/n$
 $a = 9.603$ (3) Å
 $b = 8.017$ (3) Å
 $c = 14.332$ (5) Å
 $\beta = 94.740$ (6)°

 $V = 1099.7$ (7) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 273$ (2) K
 $0.50 \times 0.50 \times 0.45$ mm

Data collection

 Bruker SMART 1K CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.973$, $T_{\max} = 0.976$

 6608 measured reflections
 2373 independent reflections
 1776 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.178$
 $S = 1.03$
 2373 reflections

 137 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Bergerhoff, 1996); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2044).

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supplementary materials

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(*E,E*)-*N*-[3-(Biphenyl-2-ylimino)butan-2-ylidene]-2-phenylaniline

H. Zou, Y. Hou, X. Yong, Y. Cen and F. Bao

Comment

As the late metal complexes are effective catalysts in the polymerization of ethylene and other olefins (Bao *et al.*, 2005), a number of studies have been directed towards the development of the late transition metal complexes (Bao, Ma *et al.*, 2006). The studies have been complemented by a report that the α -diimine ligand unit of the Ni complex is responsible for catalytic activity in the homopolymerization of ethylene (Zou *et al.*, 2005). The crystal structure of this α -diimine ligand has been obtained by our group. It was characterized by X-ray diffraction.

Experimental

α -Diimine ligands was prepared according to modified literature procedures (Bao *et al.*, 2005; Bao, Lü *et al.*, 2006; Bao, Ma *et al.*, 2006). 3-Butanedione 1.3 ml (1.27 g, 14.8 mmol) and 2-aminobiphenyl 5.00 g (29.5 mmol) were stirred for 5 h at 55°C in 25 ml of ethanol containing 1 ml formic acid. The precipitated orange solid was collected by filtration and dried. The crude product was recrystallized from a mixed solvent of petroleum aether/ethyl acetate 1:1 to give the pure ligand, yield 3.20 g, 51.04%. Anal. Calcd. for C₂₈H₂₄N₂: C, 86.56; H, 6.23; N, 7.21. Found: C, 86.48; H, 6.25; N, 7.02. Crystals suitable for X-ray structure determination were grown from a solution of the title compound in a (1:1) mixture of dichloromethane-ethanol.

Refinement

H atoms were placed in calculated positions [C—H=0.93 Å and U(H) = 1.2U_{eq}(C)] and were included in the refinement in the riding model approximation.

Figures

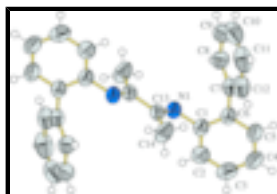


Fig. 1. View of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius and the hydrogen bond is indicated by a double-dashed line.

(*E,E*)-*N*-[3-(Biphenyl-2-ylimino)butan-2-ylidene]-2-phenylaniline

Crystal data

C₂₈H₂₄N₂

M_r = 388.49

Monoclinic, *P*2₁/*n*

*F*₀₀₀ = 412

D_x = 1.173 Mg m⁻³

Mo *K*α radiation

supplementary materials

Hall symbol: -P 2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 9.603 (3) \text{ \AA}$	Cell parameters from 775 reflections
$b = 8.017 (3) \text{ \AA}$	$\theta = 2.7\text{--}26.1^\circ$
$c = 14.332 (5) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$\beta = 94.740 (6)^\circ$	$T = 273 (2) \text{ K}$
$V = 1099.7 (7) \text{ \AA}^3$	Block, yellow
$Z = 2$	$0.50 \times 0.50 \times 0.45 \text{ mm}$

Data collection

Bruker SMART 1K CCD diffractometer	2373 independent reflections
Radiation source: fine-focus sealed tube	1776 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.029$
Detector resolution: 10 pixels mm^{-1}	$\theta_{\text{max}} = 27.0^\circ$
$T = 273(2) \text{ K}$	$\theta_{\text{min}} = 2.5^\circ$
ω scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$k = -10 \rightarrow 8$
$T_{\text{min}} = 0.973$, $T_{\text{max}} = 0.976$	$l = -15 \rightarrow 18$
6608 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.1119P)^2 + 0.1177P]$
$wR(F^2) = 0.178$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2373 reflections	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
137 parameters	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.126 (15)

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 $F^2 > 2\sigma(F^2)$ is used only for calculat-

ing 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.41183 (12)	0.12272 (16)	0.07641 (9)	0.0549 (4)
C1	0.28095 (15)	0.14069 (18)	0.11538 (11)	0.0522 (4)
C2	0.26218 (19)	0.0733 (2)	0.20274 (12)	0.0678 (5)
H2A	0.3336	0.0117	0.2340	0.081*
C3	0.1387 (2)	0.0970 (2)	0.24353 (14)	0.0766 (6)
H3A	0.1269	0.0505	0.3018	0.092*
C4	0.03264 (19)	0.1895 (2)	0.19818 (14)	0.0728 (5)
H4A	-0.0501	0.2073	0.2261	0.087*
C5	0.05000 (16)	0.2551 (2)	0.11148 (13)	0.0626 (5)
H5A	-0.0224	0.3163	0.0810	0.075*
C6	0.17315 (14)	0.23261 (18)	0.06781 (10)	0.0513 (4)
C7	0.18618 (15)	0.30173 (19)	-0.02718 (10)	0.0540 (4)
C8	0.29127 (18)	0.4124 (2)	-0.04477 (12)	0.0638 (5)
H8A	0.3572	0.4420	0.0036	0.077*
C9	0.3002 (2)	0.4798 (3)	-0.13270 (13)	0.0799 (6)
H9A	0.3708	0.5554	-0.1429	0.096*
C10	0.2048 (3)	0.4352 (3)	-0.20518 (14)	0.0936 (8)
H10A	0.2104	0.4808	-0.2644	0.112*
C11	0.1018 (3)	0.3236 (3)	-0.18970 (15)	0.0941 (8)
H11A	0.0383	0.2920	-0.2391	0.113*
C12	0.09052 (19)	0.2568 (3)	-0.10133 (13)	0.0731 (5)
H12A	0.0191	0.1820	-0.0916	0.088*
C13	0.43020 (13)	0.00418 (18)	0.02004 (10)	0.0503 (4)
C14	0.32384 (18)	-0.1253 (3)	-0.00980 (15)	0.0783 (6)
H14C	0.3624	-0.2013	-0.0526	0.117*
H14B	0.2426	-0.0724	-0.0401	0.117*
H14A	0.2982	-0.1855	0.0441	0.117*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0449 (7)	0.0577 (7)	0.0620 (8)	0.0032 (5)	0.0036 (5)	-0.0031 (6)
C1	0.0450 (7)	0.0529 (8)	0.0590 (8)	-0.0012 (6)	0.0060 (6)	-0.0063 (6)
C2	0.0647 (10)	0.0702 (10)	0.0682 (10)	0.0027 (8)	0.0049 (8)	0.0078 (8)
C3	0.0831 (13)	0.0817 (12)	0.0680 (11)	-0.0117 (10)	0.0237 (9)	0.0057 (9)
C4	0.0608 (10)	0.0759 (11)	0.0854 (12)	-0.0047 (9)	0.0285 (9)	-0.0047 (9)
C5	0.0489 (9)	0.0618 (9)	0.0783 (11)	0.0025 (7)	0.0126 (7)	-0.0076 (7)
C6	0.0464 (8)	0.0481 (8)	0.0594 (8)	-0.0015 (6)	0.0056 (6)	-0.0090 (6)
C7	0.0503 (8)	0.0545 (8)	0.0570 (8)	0.0132 (6)	0.0045 (6)	-0.0080 (6)
C8	0.0706 (10)	0.0619 (10)	0.0605 (10)	0.0030 (8)	0.0155 (7)	-0.0056 (7)
C9	0.1029 (15)	0.0716 (11)	0.0695 (11)	0.0155 (10)	0.0331 (10)	0.0031 (9)
C10	0.128 (2)	0.0970 (16)	0.0586 (11)	0.0514 (15)	0.0237 (12)	0.0052 (10)

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C11	0.1005 (16)	0.1150 (18)	0.0631 (12)	0.0464 (15)	-0.0156 (11)	-0.0194 (12)
C12	0.0634 (10)	0.0816 (12)	0.0721 (11)	0.0155 (9)	-0.0080 (8)	-0.0144 (9)
C13	0.0435 (8)	0.0497 (8)	0.0573 (8)	0.0037 (6)	0.0018 (6)	0.0011 (6)
C14	0.0592 (10)	0.0759 (12)	0.1026 (14)	-0.0153 (9)	0.0236 (9)	-0.0272 (10)

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

N1—C13	1.2691 (19)	C8—C9	1.380 (3)
N1—C1	1.424 (2)	C8—H8A	0.9300
C1—C2	1.389 (2)	C9—C10	1.374 (3)
C1—C6	1.401 (2)	C9—H9A	0.9300
C2—C3	1.378 (3)	C10—C11	1.365 (3)
C2—H2A	0.9300	C10—H10A	0.9300
C3—C4	1.378 (3)	C11—C12	1.388 (3)
C3—H3A	0.9300	C11—H11A	0.9300
C4—C5	1.372 (3)	C12—H12A	0.9300
C4—H4A	0.9300	C13—C14	1.494 (2)
C5—C6	1.395 (2)	C13—C13 ⁱ	1.503 (3)
C5—H5A	0.9300	C14—H14C	0.9600
C6—C7	1.485 (2)	C14—H14B	0.9600
C7—C8	1.383 (2)	C14—H14A	0.9600
C7—C12	1.393 (2)		
C13—N1—C1	119.94 (12)	C9—C8—H8A	119.4
C2—C1—C6	119.83 (14)	C7—C8—H8A	119.4
C2—C1—N1	119.91 (14)	C10—C9—C8	120.0 (2)
C6—C1—N1	120.19 (14)	C10—C9—H9A	120.0
C3—C2—C1	120.61 (16)	C8—C9—H9A	120.0
C3—C2—H2A	119.7	C11—C10—C9	119.61 (19)
C1—C2—H2A	119.7	C11—C10—H10A	120.2
C2—C3—C4	120.15 (17)	C9—C10—H10A	120.2
C2—C3—H3A	119.9	C10—C11—C12	120.9 (2)
C4—C3—H3A	119.9	C10—C11—H11A	119.5
C5—C4—C3	119.54 (16)	C12—C11—H11A	119.5
C5—C4—H4A	120.2	C11—C12—C7	120.0 (2)
C3—C4—H4A	120.2	C11—C12—H12A	120.0
C4—C5—C6	121.86 (16)	C7—C12—H12A	120.0
C4—C5—H5A	119.1	N1—C13—C14	125.10 (14)
C6—C5—H5A	119.1	N1—C13—C13 ⁱ	116.87 (15)
C5—C6—C1	118.00 (15)	C14—C13—C13 ⁱ	118.03 (16)
C5—C6—C7	120.13 (14)	C13—C14—H14C	109.5
C1—C6—C7	121.85 (13)	C13—C14—H14B	109.5
C8—C7—C12	118.16 (16)	H14C—C14—H14B	109.5
C8—C7—C6	121.66 (14)	C13—C14—H14A	109.5
C12—C7—C6	120.18 (16)	H14C—C14—H14A	109.5
C9—C8—C7	121.27 (18)	H14B—C14—H14A	109.5

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

Fig. 1

