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N,*N*′-(*m*-Phenylenedimethylidyne)-dianiline

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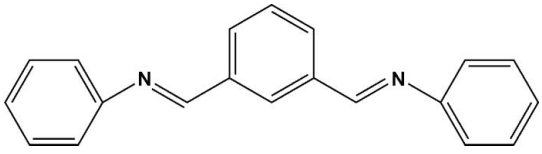
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.130; data-to-parameter ratio = 18.2.

A new Schiff base compound, $C_{20}H_{16}N_2$, was prepared by the reaction of isophthalaldehyde with aniline. The terminal phenyl rings are almost perpendicular, with a dihedral angle of 85.8 (2)°. The terminal phenyl rings make dihedral angles of 60.8 (2) and 52.5 (2)° with the central ring. Both C=N groups adopt a *trans* configuration. Adjacent pairs of centrosymmetrically related molecules are connected *via* π–π stacking interactions between their central benzene rings, with a centroid–centroid distance of 3.747 (2) Å.

Related literature

The corresponding complex 1,4-terephthalylidene-bis-*N*-aniline (Thyen & Zugenmaier, 1994), with terephthalaldehyde instead of isophthalaldehyde, is centrosymmetric, with the two parallel aniline terminal groups in a *trans* arrangement. For a review of Schiff base chemistry, see: Costamagna *et al.* (1992).



Experimental

Crystal data

$C_{20}H_{16}N_2$
M_r = 284.35
Triclinic, $P\overline{1}$
a = 7.7762 (16) Å
b = 10.301 (2) Å
c = 10.744 (2) Å
α = 79.79 (3)°
β = 78.85 (3)°
γ = 73.64 (3)°
V = 803.3 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 295 (2) K
0.38 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.973, T_{max} = 0.990
7920 measured reflections
3624 independent reflections
2738 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.130
S = 1.10
3624 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EM2001).

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supplementary materials

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N,*N*'-(*m*-Phenylenedimethylidyne)dianiline

L.-N. Zhu, S. Gao and L.-H. Huo

Comment

Schiff base complexes have been playing an important part in the area of coordination and supramolecular chemistry. The metal complexes of Schiff bases have been of interest for many years due to their homogeneous catalysis and enzymatic reactions, antibacterial activities, magnetism and molecular architectures (Costamagna *et al.*, 1992). Accordingly, we have designed and synthesized a new Schiff base complex, *viz*. 1,3-Isophthalylidene-bis(N-aniline).

The molecular structure of (I) is shown in Fig. 1. Each of the individual benzene ring is essentially planar. the terminal phenyl rings are almost perpendicular, with a relative dihedral angle of 85.8 (2) °. The terminal phenyl rings (C1—C6) and (C15—C20) make dihedral angles of 119.2 (2) and 52.5 (2) °, respectively with the central ring. Pairs of centrosymmetrically related molecules are cross-linked *via* π-π stacking interactions between the central C_6 rings of the molecules at (*x*, *y*, *z*) and (1 − *x*, 1 − *y*, 1 − *z*), with a centroid···centroid distance of 3.747 (2) Å (Fig. 2). The corresponding complex 1,4-Terephthalylidene-bis-N-aniline (Thyen & Zugenmaier, 1994), with terephthalaldehyde instead of isophthalaldehyde, is centrosymmetric with the two parallel aniline terminal groups in a *trans* arrangement and the structure does not exhibit π-π stacking.

Experimental

To a solution of isophthalaldehyde (1.34 g, 10 mmol) in ethanol was added a solution of aniline (0.93 g, 10 mmol) in ethanol. The mixture was refluxed for 2 h, and a yellow precipitate (8 mmol) was obtained. Colorless crystals were obtained by recrystallization of the material from methanol with a yield of 80%. Analysis calculated for $C_{20}H_{16}N_2$: C 84.48, H 5.67, N 9.85%. Found: C 84.44, H 5.63, N 9.89%.

Refinement

C-bound H atoms were placed in calculated positions, with phenyl C—H = 0.95 Å and methylene C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C), which were included in the refinement in a riding-model.

Figures

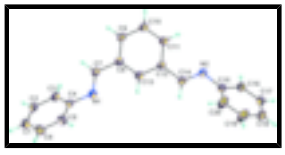

Fig. 1. A view of complex (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms drawn as spheres of arbitrary radius.

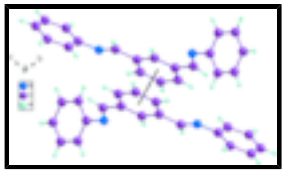

Fig. 2. A unit cell packing plot with the two molecules in the cell. *Cg*1 and *Cg*2 represent the centroids of adjacent central phenyl rings, as defined in the comment section.

N,N'-(*m*-Phenylenedimethylidyne)dianiline

Crystal data

$C_{20}H_{16}N_2$	$Z = 2$
$M_r = 284.35$	$F_{000} = 300$
Triclinic, $P\overline{1}$	$D_x = 1.176$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.7762$ (16) Å	Cell parameters from 6349 reflections
$b = 10.301$ (2) Å	$\theta = 3.0$–27.5º
$c = 10.744$ (2) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 79.79$ (3)º	$T = 295$ (2) K
$\beta = 78.85$ (3)º	Prism, colourless
$\gamma = 73.64$ (3)º	0.38 × 0.26 × 0.18 mm
$V = 803.3$ (3) Å^3	

Data collection

Rigaku RAXIS-RAPID diffractometer	3624 independent reflections
Radiation source: fine-focus sealed tube	2738 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295(2)$ K	$\theta_{min} = 3.0$º
ω scans	$h = -10 \rightarrow 9$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -13 \rightarrow 12$
$T_{min} = 0.973$, $T_{max} = 0.990$	$l = -13 \rightarrow 13$
7920 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
3624 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}

199 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.66676 (14)	0.80219 (11)	0.43392 (10)	0.0506 (3)
N2	0.27572 (14)	0.42636 (11)	0.86926 (10)	0.0494 (3)
C1	1.0361 (2)	0.99763 (16)	0.19367 (15)	0.0654 (4)
H1	1.1191	1.0410	0.1415	0.079*
C2	0.99453 (19)	0.89164 (16)	0.15464 (13)	0.0594 (4)
H2	1.0506	0.8629	0.0760	0.071*
C3	0.86986 (17)	0.82709 (14)	0.23124 (12)	0.0514 (3)
H3	0.8414	0.7560	0.2038	0.062*
C4	0.78783 (16)	0.86901 (12)	0.34905 (11)	0.0459 (3)
C5	0.83306 (19)	0.97395 (14)	0.38884 (14)	0.0584 (3)
H5	0.7815	1.0008	0.4689	0.070*
C6	0.9545 (2)	1.03902 (15)	0.31012 (16)	0.0674 (4)
H6	0.9812	1.1116	0.3363	0.081*
C7	0.53387 (16)	0.78369 (12)	0.39400 (12)	0.0463 (3)
H7	0.5145	0.8189	0.3105	0.056*
C8	0.40962 (15)	0.70868 (11)	0.47468 (11)	0.0433 (3)
C9	0.25288 (16)	0.70395 (13)	0.43283 (12)	0.0488 (3)
H9	0.2261	0.7498	0.3534	0.059*
C10	0.13722 (16)	0.63159 (14)	0.50845 (13)	0.0519 (3)
H10	0.0327	0.6295	0.4798	0.062*
C11	0.17518 (16)	0.56267 (12)	0.62576 (12)	0.0477 (3)
H11	0.0970	0.5135	0.6757	0.057*
C12	0.33100 (15)	0.56638 (12)	0.67014 (11)	0.0434 (3)
C13	0.44736 (15)	0.63837 (12)	0.59366 (11)	0.0439 (3)
H13	0.5523	0.6398	0.6221	0.053*
C14	0.37739 (17)	0.49192 (13)	0.79393 (11)	0.0484 (3)
H14	0.4857	0.4931	0.8178	0.058*
C15	0.33471 (16)	0.34699 (13)	0.98210 (12)	0.0473 (3)
C16	0.21510 (17)	0.35252 (15)	1.09537 (13)	0.0566 (3)
H16	0.0994	0.4111	1.0974	0.068*
C17	0.26643 (19)	0.27153 (15)	1.20555 (13)	0.0591 (4)
H17	0.1859	0.2780	1.2818	0.071*
C18	0.4324 (2)	0.18267 (15)	1.20450 (14)	0.0626 (4)
H18	0.4655	0.1282	1.2792	0.075*
C19	0.5502 (2)	0.1741 (2)	1.09289 (16)	0.0879 (6)
H19	0.6636	0.1122	1.0912	0.105*
C20	0.5026 (2)	0.25688 (19)	0.98157 (14)	0.0778 (5)
H20	0.5849	0.2512	0.9062	0.093*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0509 (6)	0.0530 (6)	0.0467 (6)	−0.0147 (5)	−0.0086 (4)	−0.0003 (5)
N2	0.0485 (6)	0.0539 (6)	0.0445 (6)	−0.0110 (5)	−0.0127 (4)	−0.0001 (5)
C1	0.0602 (8)	0.0676 (9)	0.0675 (9)	−0.0266 (7)	−0.0142 (7)	0.0154 (7)
C2	0.0573 (8)	0.0716 (9)	0.0455 (7)	−0.0169 (7)	−0.0095 (6)	0.0047 (6)
C3	0.0548 (7)	0.0539 (7)	0.0463 (7)	−0.0152 (6)	−0.0142 (5)	0.0007 (5)
C4	0.0447 (6)	0.0438 (6)	0.0467 (7)	−0.0082 (5)	−0.0130 (5)	0.0025 (5)
C5	0.0608 (8)	0.0530 (7)	0.0617 (8)	−0.0134 (6)	−0.0093 (6)	−0.0102 (6)
C6	0.0709 (9)	0.0538 (8)	0.0840 (11)	−0.0260 (7)	−0.0172 (8)	−0.0035 (7)
C7	0.0469 (6)	0.0446 (6)	0.0435 (6)	−0.0063 (5)	−0.0096 (5)	−0.0021 (5)
C8	0.0420 (6)	0.0397 (6)	0.0450 (6)	−0.0046 (5)	−0.0069 (5)	−0.0068 (5)
C9	0.0468 (6)	0.0505 (7)	0.0453 (7)	−0.0050 (5)	−0.0150 (5)	0.0004 (5)
C10	0.0421 (6)	0.0560 (7)	0.0578 (8)	−0.0097 (6)	−0.0181 (5)	−0.0012 (6)
C11	0.0417 (6)	0.0474 (6)	0.0520 (7)	−0.0096 (5)	−0.0092 (5)	−0.0019 (5)
C12	0.0425 (6)	0.0428 (6)	0.0423 (6)	−0.0051 (5)	−0.0087 (5)	−0.0057 (5)
C13	0.0416 (6)	0.0461 (6)	0.0450 (6)	−0.0088 (5)	−0.0107 (5)	−0.0080 (5)
C14	0.0441 (6)	0.0558 (7)	0.0450 (7)	−0.0097 (6)	−0.0121 (5)	−0.0047 (5)
C15	0.0477 (6)	0.0515 (7)	0.0432 (6)	−0.0119 (6)	−0.0131 (5)	−0.0020 (5)
C16	0.0419 (6)	0.0664 (8)	0.0553 (8)	−0.0108 (6)	−0.0071 (5)	0.0035 (6)
C17	0.0553 (8)	0.0707 (9)	0.0480 (7)	−0.0205 (7)	−0.0047 (6)	0.0048 (6)
C18	0.0698 (9)	0.0639 (8)	0.0492 (8)	−0.0114 (7)	−0.0190 (6)	0.0073 (6)
C19	0.0689 (10)	0.1005 (13)	0.0617 (10)	0.0240 (9)	−0.0132 (8)	0.0037 (9)
C20	0.0632 (9)	0.0964 (12)	0.0467 (8)	0.0143 (9)	−0.0034 (6)	−0.0009 (7)

Geometric parameters (Å, °)

N1—C7	1.2648 (16)	C9—H9	0.9300
N1—C4	1.4149 (16)	C10—C11	1.3743 (18)
N2—C14	1.2632 (17)	C10—H10	0.9300
N2—C15	1.4146 (16)	C11—C12	1.3976 (17)
C1—C6	1.371 (2)	C11—H11	0.9300
C1—C2	1.373 (2)	C12—C13	1.3849 (17)
C1—H1	0.9300	C12—C14	1.4682 (17)
C2—C3	1.3855 (19)	C13—H13	0.9300
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.3863 (18)	C15—C20	1.372 (2)
C3—H3	0.9300	C15—C16	1.3807 (18)
C4—C5	1.3825 (19)	C16—C17	1.3791 (19)
C5—C6	1.379 (2)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.355 (2)
C6—H6	0.9300	C17—H17	0.9300
C7—C8	1.4632 (17)	C18—C19	1.361 (2)
C7—H7	0.9300	C18—H18	0.9300
C8—C13	1.3936 (17)	C19—C20	1.388 (2)
C8—C9	1.3941 (17)	C19—H19	0.9300
C9—C10	1.3801 (18)	C20—H20	0.9300

C7—N1—C4	119.49 (11)	C9—C10—H10	119.7
C14—N2—C15	119.86 (11)	C10—C11—C12	120.12 (12)
C6—C1—C2	119.56 (14)	C10—C11—H11	119.9
C6—C1—H1	120.2	C12—C11—H11	119.9
C2—C1—H1	120.2	C13—C12—C11	119.18 (11)
C1—C2—C3	120.66 (14)	C13—C12—C14	119.25 (11)
C1—C2—H2	119.7	C11—C12—C14	121.54 (11)
C3—C2—H2	119.7	C12—C13—C8	121.02 (11)
C2—C3—C4	119.62 (13)	C12—C13—H13	119.5
C2—C3—H3	120.2	C8—C13—H13	119.5
C4—C3—H3	120.2	N2—C14—C12	122.46 (11)
C5—C4—C3	119.40 (12)	N2—C14—H14	118.8
C5—C4—N1	118.50 (12)	C12—C14—H14	118.8
C3—C4—N1	121.99 (12)	C20—C15—C16	118.43 (12)
C6—C5—C4	120.16 (14)	C20—C15—N2	122.31 (12)
C6—C5—H5	119.9	C16—C15—N2	119.09 (11)
C4—C5—H5	119.9	C17—C16—C15	120.27 (12)
C1—C6—C5	120.55 (14)	C17—C16—H16	119.9
C1—C6—H6	119.7	C15—C16—H16	119.9
C5—C6—H6	119.7	C18—C17—C16	121.03 (13)
N1—C7—C8	122.23 (11)	C18—C17—H17	119.5
N1—C7—H7	118.9	C16—C17—H17	119.5
C8—C7—H7	118.9	C17—C18—C19	119.27 (13)
C13—C8—C9	118.70 (11)	C17—C18—H18	120.4
C13—C8—C7	120.71 (11)	C19—C18—H18	120.4
C9—C8—C7	120.58 (11)	C18—C19—C20	120.55 (15)
C10—C9—C8	120.43 (11)	C18—C19—H19	119.7
C10—C9—H9	119.8	C20—C19—H19	119.7
C8—C9—H9	119.8	C15—C20—C19	120.41 (14)
C11—C10—C9	120.55 (12)	C15—C20—H20	119.8
C11—C10—H10	119.7	C19—C20—H20	119.8
C6—C1—C2—C3	0.6 (2)	C10—C11—C12—C14	−178.87 (11)
C1—C2—C3—C4	−0.70 (19)	C11—C12—C13—C8	1.12 (17)
C2—C3—C4—C5	−0.59 (18)	C14—C12—C13—C8	179.03 (10)
C2—C3—C4—N1	−176.67 (11)	C9—C8—C13—C12	−0.81 (17)
C7—N1—C4—C5	131.54 (13)	C7—C8—C13—C12	−179.55 (10)
C7—N1—C4—C3	−52.35 (16)	C15—N2—C14—C12	174.56 (11)
C3—C4—C5—C6	2.01 (19)	C13—C12—C14—N2	178.68 (11)
N1—C4—C5—C6	178.23 (12)	C11—C12—C14—N2	−3.47 (19)
C2—C1—C6—C5	0.9 (2)	C14—N2—C15—C20	−48.6 (2)
C4—C5—C6—C1	−2.2 (2)	C14—N2—C15—C16	136.25 (14)
C4—N1—C7—C8	176.51 (10)	C20—C15—C16—C17	1.7 (2)
N1—C7—C8—C13	−8.86 (18)	N2—C15—C16—C17	177.05 (12)
N1—C7—C8—C9	172.43 (12)	C15—C16—C17—C18	−1.8 (2)
C13—C8—C9—C10	0.39 (18)	C16—C17—C18—C19	0.3 (2)
C7—C8—C9—C10	179.13 (11)	C17—C18—C19—C20	1.1 (3)
C8—C9—C10—C11	−0.30 (19)	C16—C15—C20—C19	−0.3 (3)
C9—C10—C11—C12	0.61 (19)	N2—C15—C20—C19	−175.48 (16)

C10—C11—C12—C13	−1.01 (18)	C18—C19—C20—C15	−1.1 (3)

Fig. 1

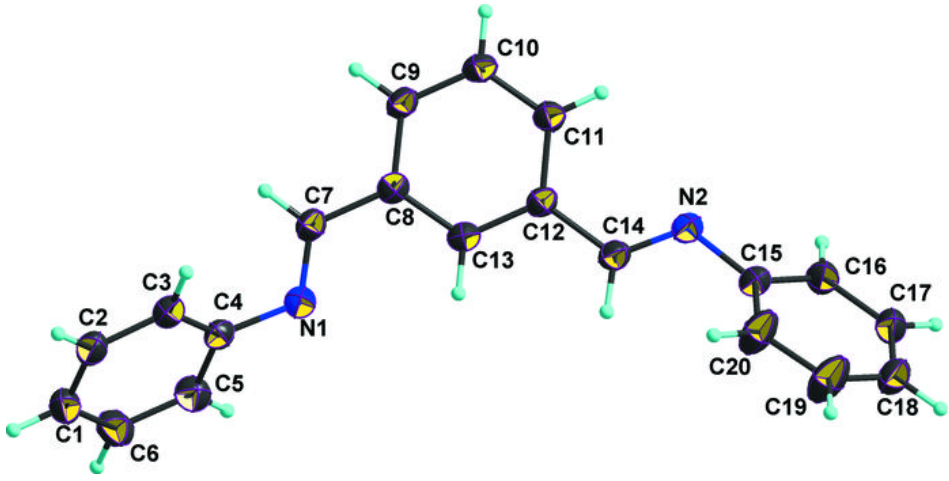

Fig. 2