organic compounds

4,4'-[Propane-1,2-diylbis(nitrilomethyl-idyne)]dibenzonitrile–4,4'-[ethane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile [0.796 (2)/0.204 (2)]

Hoong-Kun Fun,[a]* Reza Kia[a]‡ and Hadi Kargar[b]

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The title cocrystal, $0.796C_{19}H_{16}N_4 \cdot 0.204C_{18}H_{14}N_4$, is a disordered mixture of two potentially bidentate Schiff base ligands. The difference in the two components of the cocrystal is the replacement of the methyl group in the linkage between the imine N atoms in the major component of the Schiff base ligand by an H atom. The imino (C=N) functional groups are coplanar with the benzene rings (only the major component) and extend in opposite directions (both components). Intermolecular π–π interactions with a centroid-to-centroid distance of 3.7371 (8) Å are observed in the crystal packing.

Related literature

For values of bond lengths, see: Allen *et al.* (1987). For related structures, see, for example: Li *et al.* (2005); Bomfim *et al.* (2005); Glidewell *et al.* (2005, 2006); Sun *et al.* (2004); Fun, Kia & Kargar (2008); Fun, Kargar & Kia (2008).

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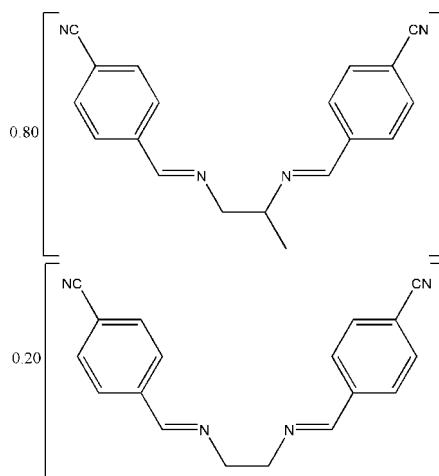
Experimental

Crystal data

$0.796C_{19}H_{16}N_4 \cdot 0.204C_{18}H_{14}N_4$	$\gamma = 67.421\ (1)°$
$M_r = 297.68$	$V = 790.15\ (3)$ Å^3
Triclinic, $P\bar{1}$	$Z = 2$
$a = 9.2370\ (2)$ Å	Mo $K\alpha$ radiation
$b = 9.7769\ (2)$ Å	$\mu = 0.08$ mm^{-1}
$c = 9.8169\ (2)$ Å	$T = 100.0\ (1)$ K
$\alpha = 81.846\ (1)°$	$0.39 \times 0.38 \times 0.27$ mm
$\beta = 75.098\ (1)°$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	17295 measured reflections
	4628 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	3746 reflections with $I > 2\sigma(I)$
$T_{min} = 0.890$, $T_{max} = 0.979$	$R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.059$	230 parameters
$wR(F^2) = 0.182$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{max} = 0.57$ e Å^{-3}
4628 reflections	$\Delta\rho_{min} = -0.48$ e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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supporting information

4,4′-[Propane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile–4,4′-[ethane-1,2-diylbis(nitrilomethylidyne)]dibenzonitrile [0.796 (2)/0.204 (2)]

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S1. Comment

Schiff bases are among the most prevalent mixed-donor ligands in the field of coordination chemistry. They play an important role in the development of catalysts and enzymatic reactions, magnetic materials and supramolecular architectures. Structures of Schiff bases derived from substituted benzaldehydes and closely related to the title compound have been reported recently (Li *et al.*, 2005; Bomfim *et al.*, 2005; Glidewell *et al.*, 2005, 2006; Sun *et al.*, 2004; Fun, Kargar & Kia, 2008; Fun, Kia & Kargar, 2008).

The title cocrystal consists of two bidentate Schiff base ligands. The bond lengths and angles in the two molecules (I, Fig. 1) are within normal ranges (Allen *et al.*, 1987). In the major component, the imino (C=N) functional groups are coplanar with the benzene rings. The difference in the two components of the co-crystal, which are disordered over two sites, is the replacement of the methyl group in the major component by a hydrogen atom in the linkage between the imino N atoms. The ratio of the refined site occupancy factors of the major and minor components is 0.796 (2)/0.204 (2). The short distance between the centroids of the six-membered rings indicates the existence of π-π interactions (Fig. 2), with a $Cg1 \cdots Cg1$ distance of 3.7371 (8) Å (symmetry code: -*x*, -*y*, 2 - *z*; $Cg1$ is the centroid of the C11–C16 benzene ring).

S2. Experimental

The synthetic method has been described previously (Fun, Kargar & Kia, 2008). Single crystals suitable for *X*-ray diffraction were obtained by evaporation of an ethanol solution at room temperature.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.98 Å. The U_{iso} values were constrained to be 1.5U_{eq} of the carrier atom for the methyl H atoms and 1.2U_{eq} for the remaining H atoms. A rotating-group model was used for the methyl groups. Incorrect bond lengths of the methylene bridge, plus the presence of large peaks in the difference Fourier map near to the methylene bridge, led us to suspect positional disorder of this segment of the title compound. The refined ratio of the site-occupany factors for the disorder parts is 0.796 (2)/0.204 (2).
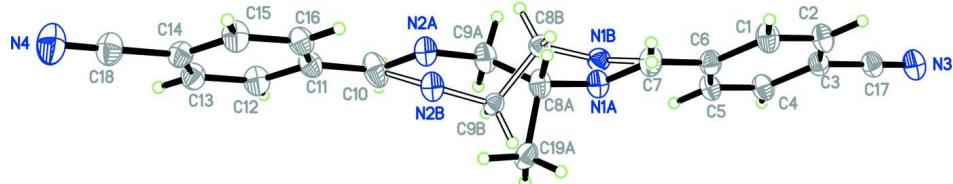
Figure 1

The molecular structure of the title cocrystal, with atom labels and 50% probability ellipsoids for non-H atoms. Open bonds indicate the minor component.
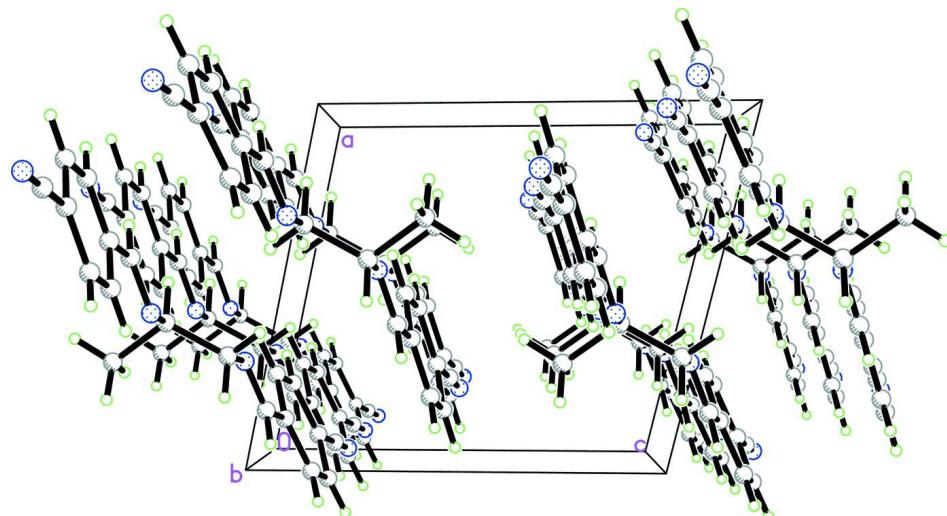
Figure 2

The crystal packing of the major component of (I), viewed down the *b*-axis.

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Crystal data

$0.796C_{19}H_{16}N_4 \cdot 0.204C_{18}H_{14}N_4$	$Z = 2$
$M_r = 297.68$	$F(000) = 313$
Triclinic, $P\overline{1}$	$D_x = 1.251$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.2370$ (2) Å	Cell parameters from 6569 reflections
$b = 9.7769$ (2) Å	$\theta = 3.2$–30.8°
$c = 9.8169$ (2) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 81.846$ (1)°	$T = 100$ K
$\beta = 75.098$ (1)°	Block, colourless
$\gamma = 67.421$ (1)°	$0.39 \times 0.38 \times 0.27$ mm
$V = 790.15$ (3) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
Radiation source: fine-focus sealed tube	$T_{min} = 0.890$, $T_{max} = 0.979$
Graphite monochromator	17295 measured reflections
φ and ω scans	4628 independent reflections
	3746 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\text{max}} = 30.1°$, $\theta_{\text{min}} = 2.2°$

$h = -13 \rightarrow 13$

$k = -13 \rightarrow 13$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.059$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.182$	
$S = 1.05$	H-atom parameters constrained
4628 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0996P)^2 + 0.2311P]$
230 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{\text{max}} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{max}} = 0.57$ e Å^{-3}
	$\Delta\rho_{\text{min}} = -0.48$ e Å^{-3}

Special details

Experimental. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1A	0.44472 (19)	0.58449 (16)	0.76563 (18)	0.0277 (3)	0.796 (2)
N2A	0.31537 (17)	0.28586 (16)	0.96983 (15)	0.0294 (3)	0.796 (2)
C8A	0.41965 (19)	0.44248 (17)	0.78683 (17)	0.0276 (3)	0.796 (2)
H8AA	0.5235	0.3602	0.7675	0.033*	0.796 (2)
C9A	0.3328 (2)	0.42957 (19)	0.93985 (17)	0.0311 (4)	0.796 (2)
H9AA	0.3933	0.4409	1.0021	0.037*	0.796 (2)
H9AB	0.2275	0.5079	0.9569	0.037*	0.796 (2)
C19A	0.3162 (2)	0.44326 (18)	0.68371 (15)	0.0302 (4)	0.796 (2)
H19A	0.3770	0.4426	0.5883	0.045*	0.796 (2)
H19B	0.2204	0.5308	0.6954	0.045*	0.796 (2)
H19C	0.2873	0.3569	0.7039	0.045*	0.796 (2)
N1B	0.4751 (7)	0.5817 (7)	0.8069 (6)	0.0236 (13)*	0.204 (2)
N2B	0.2894 (7)	0.2948 (6)	0.8959 (6)	0.0294 (3)	0.204 (2)
C8B	0.4619 (7)	0.4375 (6)	0.8536 (6)	0.0225 (11)*	0.204 (2)
H8BA	0.4726	0.4144	0.9508	0.027*	0.204 (2)
H8BB	0.5478	0.3612	0.7959	0.027*	0.204 (2)
C9B	0.2974 (6)	0.4397 (6)	0.8414 (6)	0.0203 (10)	0.204 (2)
H9BA	0.2106	0.5179	0.8962	0.024*	0.204 (2)
H9BB	0.2881	0.4571	0.7437	0.024*	0.204 (2)
N3	0.77232 (14)	1.20704 (14)	0.53274 (13)	0.0356 (3)	
N4	0.04293 (17)	−0.36229 (15)	1.22228 (16)	0.0481 (4)	

C1	0.77783 (15)	0.70764 (15)	0.59144 (14)	0.0310 (3)	
H1A	0.8552	0.6156	0.5652	0.037*	
C2	0.81727 (15)	0.83368 (15)	0.55783 (13)	0.0301 (3)	
H2A	0.9207	0.8263	0.5101	0.036*	
C3	0.70001 (14)	0.97147 (14)	0.59648 (12)	0.0250 (2)	
C4	0.54475 (14)	0.98285 (14)	0.66949 (13)	0.0281 (3)	
H4A	0.4671	1.0749	0.6957	0.034*	
C5	0.50763 (14)	0.85626 (14)	0.70243 (13)	0.0274 (3)	
H5A	0.4043	0.8635	0.7507	0.033*	
C6	0.62345 (14)	0.71778 (14)	0.66410 (12)	0.0248 (2)	
C7	0.58542 (16)	0.58172 (14)	0.69901 (14)	0.0302 (3)	
H7A	0.6682	0.4882	0.6713	0.036*	0.796 (2)
H7B	0.6427	0.4971	0.6419	0.036*	0.204 (2)
C10	0.18277 (17)	0.28390 (16)	1.04041 (17)	0.0379 (3)	
H10A	0.0979	0.3754	1.0711	0.045*	0.796 (2)
H10B	0.1389	0.3631	1.1042	0.045*	0.204 (2)
C11	0.15451 (14)	0.14439 (14)	1.07915 (13)	0.0269 (3)	
C12	0.00891 (15)	0.14545 (14)	1.16669 (14)	0.0309 (3)	
H12A	−0.0691	0.2345	1.2005	0.037*	
C13	−0.02034 (15)	0.01501 (14)	1.20368 (13)	0.0285 (3)	
H13A	−0.1174	0.0161	1.2625	0.034*	
C14	0.09638 (15)	−0.11766 (14)	1.15229 (13)	0.0269 (3)	
C15	0.24291 (15)	−0.12015 (15)	1.06462 (14)	0.0316 (3)	
H15A	0.3205	−0.2092	1.0303	0.038*	
C16	0.27163 (14)	0.01010 (14)	1.02930 (13)	0.0283 (3)	
H16A	0.3695	0.0086	0.9720	0.034*	
C17	0.73983 (15)	1.10277 (15)	0.56153 (13)	0.0281 (3)	
C18	0.06622 (17)	−0.25355 (16)	1.19090 (15)	0.0348 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1A	0.0290 (7)	0.0270 (7)	0.0282 (7)	−0.0139 (5)	−0.0013 (6)	−0.0031 (5)
N2A	0.0304 (6)	0.0287 (6)	0.0298 (7)	−0.0149 (5)	−0.0010 (5)	−0.0024 (5)
C8A	0.0276 (7)	0.0234 (7)	0.0311 (8)	−0.0119 (6)	−0.0002 (6)	−0.0034 (6)
C9A	0.0340 (8)	0.0303 (8)	0.0313 (8)	−0.0176 (6)	0.0008 (6)	−0.0062 (6)
C19A	0.0537 (10)	0.0276 (7)	0.0222 (7)	−0.0273 (7)	−0.0126 (6)	0.0023 (5)
N2B	0.0304 (6)	0.0287 (6)	0.0298 (7)	−0.0149 (5)	−0.0010 (5)	−0.0024 (5)
C9B	0.024 (2)	0.016 (2)	0.021 (2)	−0.0076 (19)	−0.0053 (18)	0.0005 (18)
N3	0.0337 (6)	0.0363 (6)	0.0387 (6)	−0.0187 (5)	0.0002 (5)	−0.0055 (5)
N4	0.0457 (7)	0.0340 (7)	0.0585 (8)	−0.0165 (6)	0.0000 (6)	0.0008 (6)
C1	0.0258 (6)	0.0283 (6)	0.0341 (6)	−0.0090 (5)	0.0027 (5)	−0.0060 (5)
C2	0.0239 (5)	0.0335 (7)	0.0312 (6)	−0.0127 (5)	0.0020 (4)	−0.0046 (5)
C3	0.0253 (5)	0.0294 (6)	0.0229 (5)	−0.0134 (5)	−0.0033 (4)	−0.0031 (4)
C4	0.0235 (5)	0.0265 (6)	0.0325 (6)	−0.0096 (4)	−0.0006 (4)	−0.0051 (5)
C5	0.0225 (5)	0.0294 (6)	0.0298 (6)	−0.0116 (5)	−0.0006 (4)	−0.0036 (5)
C6	0.0252 (5)	0.0268 (6)	0.0219 (5)	−0.0112 (4)	−0.0011 (4)	−0.0029 (4)
C7	0.0304 (6)	0.0258 (6)	0.0308 (6)	−0.0108 (5)	0.0010 (5)	−0.0025 (5)

C10	0.0293 (6)	0.0273 (6)	0.0558 (9)	−0.0129 (5)	0.0018 (6)	−0.0112 (6)
C11	0.0248 (5)	0.0261 (6)	0.0312 (6)	−0.0105 (4)	−0.0043 (4)	−0.0055 (4)
C12	0.0260 (6)	0.0257 (6)	0.0360 (6)	−0.0066 (5)	0.0000 (5)	−0.0066 (5)
C13	0.0236 (5)	0.0305 (6)	0.0283 (6)	−0.0094 (5)	−0.0015 (4)	−0.0008 (5)
C14	0.0269 (6)	0.0263 (6)	0.0263 (5)	−0.0094 (5)	−0.0046 (4)	−0.0005 (4)
C15	0.0271 (6)	0.0265 (6)	0.0358 (6)	−0.0072 (5)	0.0004 (5)	−0.0057 (5)
C16	0.0232 (5)	0.0299 (6)	0.0303 (6)	−0.0100 (5)	−0.0006 (4)	−0.0054 (5)
C17	0.0256 (5)	0.0330 (6)	0.0269 (6)	−0.0134 (5)	−0.0013 (4)	−0.0054 (5)
C18	0.0326 (6)	0.0304 (7)	0.0372 (7)	−0.0113 (5)	−0.0012 (5)	−0.0005 (5)

Geometric parameters (Å, º)

N1A—C7	1.2878 (18)	C2—C3	1.3947 (18)
N1A—C8A	1.4714 (19)	C2—H2A	0.9300
N2A—C10	1.2484 (18)	C3—C4	1.3979 (16)
N2A—C9A	1.455 (2)	C3—C17	1.4400 (16)
C8A—C9A	1.523 (2)	C4—C5	1.3818 (16)
C8A—C19A	1.558 (2)	C4—H4A	0.9300
C8A—H8AA	0.9800	C5—C6	1.3944 (17)
C9A—H9AA	0.9700	C5—H5A	0.9300
C9A—H9AB	0.9700	C6—C7	1.4758 (16)
C19A—H19A	0.9600	C7—H7A	0.9600
C19A—H19B	0.9600	C7—H7B	0.9600
C19A—H19C	0.9600	C10—C11	1.4658 (17)
N1B—C7	1.267 (6)	C10—H10A	0.9600
N1B—C8B	1.460 (8)	C10—H10B	0.9600
N2B—C9B	1.464 (7)	C11—C12	1.3945 (17)
N2B—C10	1.521 (6)	C11—C16	1.3975 (17)
C8B—C9B	1.546 (8)	C12—C13	1.3834 (17)
C8B—H8BA	0.9700	C12—H12A	0.9300
C8B—H8BB	0.9700	C13—C14	1.3897 (17)
C9B—H9BA	0.9700	C13—H13A	0.9300
C9B—H9BB	0.9700	C14—C15	1.3982 (17)
N3—C17	1.1484 (17)	C14—C18	1.4400 (18)
N4—C18	1.1489 (19)	C15—C16	1.3781 (17)
C1—C2	1.3883 (17)	C15—H15A	0.9300
C1—C6	1.3930 (16)	C16—H16A	0.9300
C1—H1A	0.9300		
C7—N1A—C8A	116.77 (13)	C1—C6—C5	119.43 (11)
C10—N2A—C9A	117.17 (13)	C1—C6—C7	119.38 (11)
N1A—C8A—C9A	107.68 (13)	C5—C6—C7	121.19 (10)
N1A—C8A—C19A	108.24 (13)	N1B—C7—N1A	24.5 (2)
C9A—C8A—C19A	111.02 (13)	N1B—C7—C6	117.3 (3)
N1A—C8A—H8AA	110.0	N1A—C7—C6	122.07 (12)
C9A—C8A—H8AA	110.0	N1B—C7—H7A	117.8
C19A—C8A—H8AA	110.0	N1A—C7—H7A	119.0
N2A—C9A—C8A	110.09 (13)	C6—C7—H7A	119.0

N2A—C9A—H9AA	109.6	N1B—C7—H7B	121.9
C8A—C9A—H9AA	109.6	N1A—C7—H7B	111.9
N2A—C9A—H9AB	109.6	C6—C7—H7B	120.8
C8A—C9A—H9AB	109.6	H7A—C7—H7B	23.9
H9AA—C9A—H9AB	108.2	N2A—C10—C11	121.33 (13)
C7—N1B—C8B	115.5 (5)	N2A—C10—N2B	31.9 (2)
C9B—N2B—C10	118.6 (4)	C11—C10—N2B	116.6 (2)
N1B—C8B—C9B	110.0 (5)	N2A—C10—H10A	119.5
N1B—C8B—H8BA	109.7	C11—C10—H10A	119.2
C9B—C8B—H8BA	109.7	N2B—C10—H10A	114.8
N1B—C8B—H8BB	109.7	N2A—C10—H10B	107.4
C9B—C8B—H8BB	109.7	C11—C10—H10B	121.7
H8BA—C8B—H8BB	108.2	N2B—C10—H10B	121.8
N2B—C9B—C8B	107.0 (4)	H10A—C10—H10B	32.0
N2B—C9B—H9BA	110.3	C12—C11—C16	119.49 (11)
C8B—C9B—H9BA	110.3	C12—C11—C10	119.68 (11)
N2B—C9B—H9BB	110.3	C16—C11—C10	120.83 (11)
C8B—C9B—H9BB	110.3	C13—C12—C11	120.51 (11)
H9BA—C9B—H9BB	108.6	C13—C12—H12A	119.7
C2—C1—C6	120.64 (11)	C11—C12—H12A	119.7
C2—C1—H1A	119.7	C12—C13—C14	119.49 (11)
C6—C1—H1A	119.7	C12—C13—H13A	120.3
C1—C2—C3	119.28 (11)	C14—C13—H13A	120.3
C1—C2—H2A	120.4	C13—C14—C15	120.52 (12)
C3—C2—H2A	120.4	C13—C14—C18	119.56 (11)
C2—C3—C4	120.53 (11)	C15—C14—C18	119.92 (11)
C2—C3—C17	119.61 (10)	C16—C15—C14	119.61 (11)
C4—C3—C17	119.86 (11)	C16—C15—H15A	120.2
C5—C4—C3	119.44 (11)	C14—C15—H15A	120.2
C5—C4—H4A	120.3	C15—C16—C11	120.37 (11)
C3—C4—H4A	120.3	C15—C16—H16A	119.8
C4—C5—C6	120.68 (11)	C11—C16—H16A	119.8
C4—C5—H5A	119.7	N3—C17—C3	179.50 (14)
C6—C5—H5A	119.7	N4—C18—C14	179.53 (16)
C7—N1A—C8A—C9A	134.28 (16)	C1—C6—C7—N1B	152.5 (3)
C7—N1A—C8A—C19A	−105.62 (18)	C5—C6—C7—N1B	−27.5 (4)
C10—N2A—C9A—C8A	−136.91 (16)	C1—C6—C7—N1A	−179.80 (14)
N1A—C8A—C9A—N2A	−175.76 (13)	C5—C6—C7—N1A	0.2 (2)
C19A—C8A—C9A—N2A	65.92 (17)	C9A—N2A—C10—C11	−178.46 (13)
C7—N1B—C8B—C9B	−116.7 (5)	C9A—N2A—C10—N2B	90.8 (4)
C10—N2B—C9B—C8B	105.6 (5)	C9B—N2B—C10—N2A	−83.9 (6)
N1B—C8B—C9B—N2B	−177.4 (5)	C9B—N2B—C10—C11	168.8 (4)
C6—C1—C2—C3	−0.6 (2)	N2A—C10—C11—C12	175.33 (15)
C1—C2—C3—C4	0.61 (19)	N2B—C10—C11—C12	−148.5 (3)
C1—C2—C3—C17	−179.77 (11)	N2A—C10—C11—C16	−4.8 (2)
C2—C3—C4—C5	−0.45 (19)	N2B—C10—C11—C16	31.4 (3)
C17—C3—C4—C5	179.94 (11)	C16—C11—C12—C13	−0.31 (19)

C3—C4—C5—C6	0.25 (19)	C10—C11—C12—C13	179.60 (12)
C2—C1—C6—C5	0.38 (19)	C11—C12—C13—C14	−0.35 (19)
C2—C1—C6—C7	−179.66 (11)	C12—C13—C14—C15	0.44 (19)
C4—C5—C6—C1	−0.22 (19)	C12—C13—C14—C18	179.89 (12)
C4—C5—C6—C7	179.83 (11)	C13—C14—C15—C16	0.1 (2)
C8B—N1B—C7—N1A	83.2 (8)	C18—C14—C15—C16	−179.31 (12)
C8B—N1B—C7—C6	−168.7 (4)	C14—C15—C16—C11	−0.8 (2)
C8A—N1A—C7—N1B	−97.6 (8)	C12—C11—C16—C15	0.90 (19)
C8A—N1A—C7—C6	176.59 (13)	C10—C11—C16—C15	−179.01 (12)