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N-Phenyl-*N*-{4-[5-(4-pyridyl)-1,3,4-oxadiazol-2-yl]phenyl}aniline

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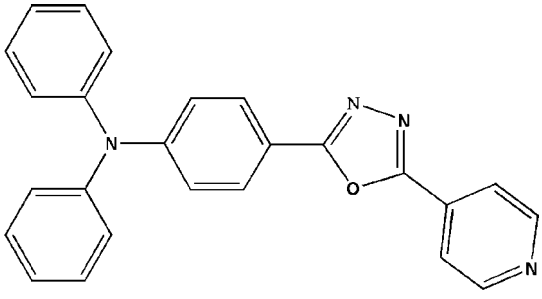
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.083; data-to-parameter ratio = 7.4.

The title compound, $C_{25}H_{18}N_4O$, is a non-planar bipolar ligand containing triphenylamine and 1,3,4-oxadiazole units. In the molecule, the benzene ring, the 1,3,4-oxadiazole ring, and the pyridine ring are twisted slightly with respect to each other [dihedral angle between the benzene and 1,3,4-oxadiazole rings = 9.4 (4) and between the 1,3,4-oxadiazole and pyridine rings = 3.0 (4)°]. Moreover, the dihedral angles between the two phenyl rings and the benzene ring are 88.2 (4) and 113.3 (4)°, and that between the two phenyl rings is 67.9 (4)°. The closest distances between the pyridine ring and the 1,3,4-oxadiazole and benzene rings in adjacent molecules are 3.316 and 3.363 Å, respectively, indicating the existence of π–π interactions.

Related literature

For related literature, see: Tang *et al.* (1987); Yeh *et al.* (2005); Xiang *et al.* (2006); Chan *et al.* (1999); Gong *et al.* (1998); Tamoto *et al.* (1997).



Experimental

Crystal data

$C_{25}H_{18}N_4O$
M_r = 390.43
Orthorhombic, $Pna2_1$
a = 10.7125 (9) Å
b = 14.1797 (12) Å
c = 12.7835 (11) Å
V = 1941.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
0.40 × 0.30 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.98
10383 measured reflections
2015 independent reflections
1655 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.083
S = 0.99
2015 reflections
271 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); 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: BG2156).

References

Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison,Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
Chan, W. K., Ng, P. K., Gong, X. & Hou, S. J. (1999). *Appl. Phys. Lett.* **75**, 3920–3922.
Gong, X., Ng, P. K. & Chan, W. K. (1998). *Adv. Mater.* **10**, 1337–1340.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. Version 2.03. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tamoto, N., Adachi, C. & Nagai, K. (1997). *Chem. Mater.* **9**, 1077–1085.
Tang, C. W. & Vanslyke, S. A. (1987). *Appl. Phys. Lett.* **51**, 913–915.
Xiang, N. J., Lee, T. H., Gong, M. L., Tong, K. L., So, S. K. & Leung, L. M. (2006). *Synth. Met.* **156**, 270–275.
Yeh, S. J., Wu, M. F., Chen, C. T., Song, Y. H., Chi, Y., Ho, M. H., Hsu, S. F. & Chen, C. H. (2005). *Adv. Mater.* **17**, 285–289.

supplementary materials

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N-Phenyl-*N*-{4-[5-(4-pyridyl)-1,3,4-oxadiazol-2-yl]phenyl}aniline

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Comment

Organic light-emitting diodes (OLEDs) have attracted considerable attentions due to potentially practical applications in large-area flat-panel display technologies, as well as to their numerous advantages, such as low cost, light weight, fast response, wide-viewing-angle, and compatibility with flexible substrates (Tang *et al.*, 1987; Yeh *et al.*, 2005).

It is well known that OLED produces light *via* recombination of electrons and holes, which are injected from electrodes on opposite sides of the device. Furthermore, the balance between the injection and transportation of electron and hole carriers leads to a high luminescence efficiency. Because triphenylamine and the 1,3,4-oxadiazol group possess good properties of hole transportation and electron deficiency, respectively, the compound containing these two groups should be of an increased electron affinity and transporting properties, resulting in a more balanced charge recombination in the emissive layer (Xiang *et al.*, 2006; Chan *et al.*, 1999; Gong *et al.*, 1998). In this contribution, we have synthesized the title compound, $C_{25}H_{18}N_4O$, with both a triphenylamine and a 1,3,4-oxadiazol moieties. This compound emits bright blue-green light under excitation of UV light, which implies its potential application in OLEDs.

The molecular skeleton of the title compound is non-planar (Fig.1), with the benzene (A), the 1,3,4-oxadiazol (B) and the pyridine (C) rings being slightly twisted with respect to each other (dihedral angles: (A),(B): 9.4 (4)°; (B),(C): 3.0 (4)°). Between the two adjacent molecules, the closest distances of C3-to-C7 and C4-to-C9 are 3.316 and 3.363 Å, respectively, indicating the existence of π–π interactions. (Fig 2).

Experimental

The title compound was synthesized *via* a tetrazole intermediate pathway. Amongst, the 4-tetrazoyltriphenylamine was prepared according to the procedures described elsewhere (Tamoto *et al.*, 1997).

Firstly, the 150 ml water solution of 4-phenylpyridine (1 ml) and KMnO4 (3.16 g) was heated for 12 h. After removal of brown precipitate by filtration, the addition of concentrated hydrochloric acid into solution led to the deposition of white crystals. This solid was filtered, washed with water, and dried in the vacuo, and then was refluxed with thionyl chloride (15 ml) for 5 h. Isonicotinoyl chloride could be achieved by removing the solution by rotary evaporation.

A mixture of isonicotinoyl chloride (0.14 g), 4-tetrazolytriphenylamine (0.31 g), and dry pyridine (30 ml) was refluxed for one day under nitrogen atmosphere. After cooling, the reaction mixture was poured into water, and then filtered to collect the solid. The crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1/5, *v*/*v*) as the eluent. Crystals suitable for X-ray diffraction study were obtained by slow evaporation of ethyl acetate/petroleum ether (1/5, *v*/*v*) solution.

Refinement

All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å, U_{iso} = 1.2U_{eq} (C). In the absence of significant anomalous scattering effects Friedel pairs have been merged

Figures

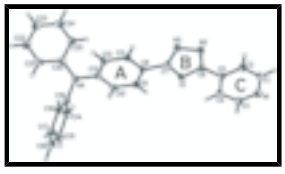


Fig. 1. A view of the molecule of (I). Displacement ellipsoids drawn at a 30% probability level. H atoms omitted for clarity.

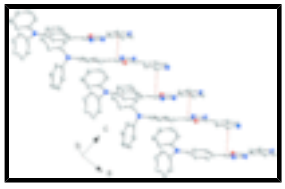


Fig. 2. Packing view of (I) showing stacking interactions between neighbouring molecules. H atoms omitted for clarity.

N-Phenyl-*N*-{4-[5-(4-pyridyl)-1,3,4-oxadiazol-2-yl]phenyl}aniline

Crystal data

$C_{25}H_{18}N_4O$	F_{000} = 816
M_r = 390.43	D_x = 1.336 Mg m^{-3}
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 2767 reflections
a = 10.7125 (9) Å	θ = 1.0–26.1°
b = 14.1797 (12) Å	μ = 0.08 mm^{-1}
c = 12.7835 (11) Å	*T* = 291 (2) K
V = 1941.8 (3) Å^3	Block, yellow
Z = 4	0.40 × 0.30 × 0.25 mm

Data collection

Bruker APEX CCD area-detector diffractometer	2015 independent reflections
Radiation source: fine-focus sealed tube	1655 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
T = 291(2) K	θ_{max} = 26.1°
ω scans	θ_{min} = 2.1°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −13→13
T_{min} = 0.970, T_{max} = 0.98	*k* = −9→17
10383 measured reflections	*l* = −15→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.037P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.083$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.99$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
2015 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
271 parameters	Extinction correction: none
1 restraint	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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 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}
C1	1.5156 (3)	0.7596 (2)	1.1070 (3)	0.0377 (8)
H1	1.5784	0.7860	1.1479	0.045*
C2	1.4338 (3)	0.8198 (2)	1.0564 (2)	0.0342 (8)
H2	1.4424	0.8849	1.0627	0.041*
C3	1.4171 (3)	0.6299 (2)	1.0426 (3)	0.0388 (8)
H3	1.4105	0.5647	1.0374	0.047*
C4	1.3304 (3)	0.6843 (2)	0.9899 (3)	0.0349 (7)
H4	1.2674	0.6561	0.9508	0.042*
C5	1.3393 (3)	0.7817 (2)	0.9964 (3)	0.0295 (7)
C6	1.2545 (3)	0.8435 (2)	0.9402 (2)	0.0282 (7)
C7	1.1064 (3)	0.8840 (2)	0.8379 (2)	0.0288 (7)
C8	1.0009 (3)	0.8726 (2)	0.7671 (2)	0.0260 (7)
C9	0.9482 (3)	0.7848 (2)	0.7485 (2)	0.0307 (7)
H9	0.9841	0.7311	0.7775	0.037*
C10	0.8425 (3)	0.7771 (2)	0.6870 (2)	0.0311 (8)
H10	0.8072	0.7181	0.6751	0.037*

C11	0.9489 (3)	0.9523 (2)	0.7205 (2)	0.0302 (7)
H11	0.9854	1.0110	0.7307	0.036*
C12	0.8434 (3)	0.9442 (2)	0.6590 (2)	0.0314 (7)
H12	0.8089	0.9976	0.6282	0.038*
C13	0.7889 (3)	0.8566 (2)	0.6432 (2)	0.0302 (7)
C14	0.7720 (3)	0.8032 (2)	0.4179 (3)	0.0401 (8)
H14	0.8247	0.8550	0.4234	0.048*
C15	0.7824 (3)	0.7427 (3)	0.3339 (3)	0.0466 (9)
H15	0.8437	0.7531	0.2837	0.056*
C16	0.7030 (3)	0.6671 (3)	0.3236 (3)	0.0439 (9)
H16	0.7097	0.6268	0.2665	0.053*
C17	0.6136 (3)	0.6518 (2)	0.3988 (3)	0.0401 (8)
H17	0.5591	0.6012	0.3917	0.048*
C18	0.6034 (3)	0.7103 (2)	0.4850 (3)	0.0362 (8)
H18	0.5436	0.6984	0.5361	0.043*
C19	0.6827 (3)	0.7865 (2)	0.4944 (3)	0.0300 (7)
C20	0.5715 (3)	0.9019 (2)	0.6056 (2)	0.0303 (7)
C21	0.4767 (3)	0.9129 (2)	0.5323 (3)	0.0352 (8)
H21	0.4856	0.8871	0.4658	0.042*
C22	0.3683 (3)	0.9621 (2)	0.5579 (3)	0.0422 (9)
H22	0.3058	0.9691	0.5080	0.051*
C23	0.3527 (3)	1.0006 (2)	0.6560 (3)	0.0431 (9)
H23	0.2795	1.0324	0.6730	0.052*
C24	0.4465 (3)	0.9913 (2)	0.7281 (3)	0.0409 (8)
H24	0.4373	1.0186	0.7938	0.049*
C25	0.5545 (3)	0.9421 (2)	0.7050 (3)	0.0336 (7)
H25	0.6163	0.9357	0.7556	0.040*
N1	1.5097 (2)	0.66508 (19)	1.1004 (2)	0.0380 (7)
N2	1.2517 (2)	0.93454 (17)	0.9404 (2)	0.0348 (6)
N3	1.1540 (2)	0.96137 (17)	0.8743 (2)	0.0351 (6)
N4	0.6774 (2)	0.84778 (18)	0.58321 (19)	0.0327 (6)
O1	1.16472 (18)	0.80569 (14)	0.87666 (16)	0.0305 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0346 (19)	0.041 (2)	0.0379 (19)	−0.0005 (16)	−0.0046 (16)	−0.0011 (16)
C2	0.0351 (18)	0.0318 (18)	0.0356 (18)	−0.0032 (14)	−0.0042 (15)	−0.0010 (15)
C3	0.045 (2)	0.0301 (18)	0.042 (2)	0.0010 (15)	0.0019 (17)	0.0038 (16)
C4	0.0359 (18)	0.0350 (19)	0.0339 (17)	0.0002 (15)	−0.0024 (16)	−0.0048 (16)
C5	0.0289 (16)	0.0333 (18)	0.0264 (15)	0.0002 (14)	0.0040 (14)	−0.0003 (15)
C6	0.0277 (16)	0.0311 (18)	0.0259 (15)	−0.0001 (14)	0.0001 (13)	−0.0026 (15)
C7	0.0333 (17)	0.0258 (17)	0.0272 (16)	0.0017 (14)	0.0043 (14)	0.0007 (14)
C8	0.0293 (16)	0.0286 (16)	0.0202 (15)	0.0015 (13)	0.0023 (13)	−0.0012 (13)
C9	0.0405 (18)	0.0240 (16)	0.0276 (17)	0.0045 (14)	−0.0001 (15)	0.0010 (14)
C10	0.0401 (19)	0.0235 (16)	0.0298 (17)	−0.0036 (15)	0.0019 (14)	−0.0060 (14)
C11	0.0370 (18)	0.0215 (16)	0.0320 (17)	−0.0020 (13)	−0.0016 (14)	−0.0014 (14)
C12	0.0404 (19)	0.0246 (17)	0.0290 (17)	0.0033 (14)	−0.0048 (15)	−0.0013 (14)

C13	0.0331 (18)	0.0319 (18)	0.0255 (16)	0.0032 (14)	−0.0013 (14)	−0.0046 (14)
C14	0.039 (2)	0.043 (2)	0.039 (2)	−0.0064 (16)	−0.0003 (16)	−0.0032 (17)
C15	0.045 (2)	0.061 (3)	0.0339 (19)	−0.0094 (19)	0.0065 (17)	−0.0104 (19)
C16	0.046 (2)	0.051 (2)	0.0353 (19)	0.0038 (18)	−0.0044 (17)	−0.0171 (18)
C17	0.042 (2)	0.0353 (19)	0.043 (2)	−0.0031 (16)	−0.0064 (17)	−0.0119 (17)
C18	0.0325 (17)	0.043 (2)	0.0335 (17)	−0.0034 (15)	0.0020 (15)	−0.0056 (17)
C19	0.0282 (16)	0.0310 (17)	0.0308 (16)	0.0034 (14)	−0.0041 (14)	−0.0037 (15)
C20	0.0330 (18)	0.0243 (16)	0.0337 (17)	−0.0055 (14)	0.0009 (14)	0.0037 (14)
C21	0.0392 (19)	0.0337 (18)	0.0326 (18)	−0.0050 (15)	0.0013 (15)	0.0010 (15)
C22	0.038 (2)	0.0335 (19)	0.055 (2)	−0.0006 (16)	−0.0036 (17)	0.0073 (19)
C23	0.038 (2)	0.037 (2)	0.054 (2)	0.0032 (16)	0.0106 (18)	0.0001 (18)
C24	0.047 (2)	0.0340 (19)	0.042 (2)	0.0004 (17)	0.0142 (18)	−0.0038 (16)
C25	0.0373 (19)	0.0295 (17)	0.0341 (18)	−0.0020 (15)	0.0022 (15)	−0.0010 (15)
N1	0.0404 (16)	0.0352 (16)	0.0384 (16)	0.0037 (14)	−0.0030 (14)	0.0026 (14)
N2	0.0363 (15)	0.0314 (15)	0.0366 (15)	0.0009 (12)	−0.0068 (13)	0.0016 (13)
N3	0.0356 (15)	0.0306 (15)	0.0389 (15)	0.0001 (12)	−0.0070 (13)	−0.0010 (13)
N4	0.0290 (14)	0.0345 (15)	0.0346 (15)	0.0025 (12)	−0.0057 (12)	−0.0114 (13)
O1	0.0343 (12)	0.0282 (12)	0.0291 (11)	0.0017 (9)	−0.0038 (10)	−0.0009 (10)

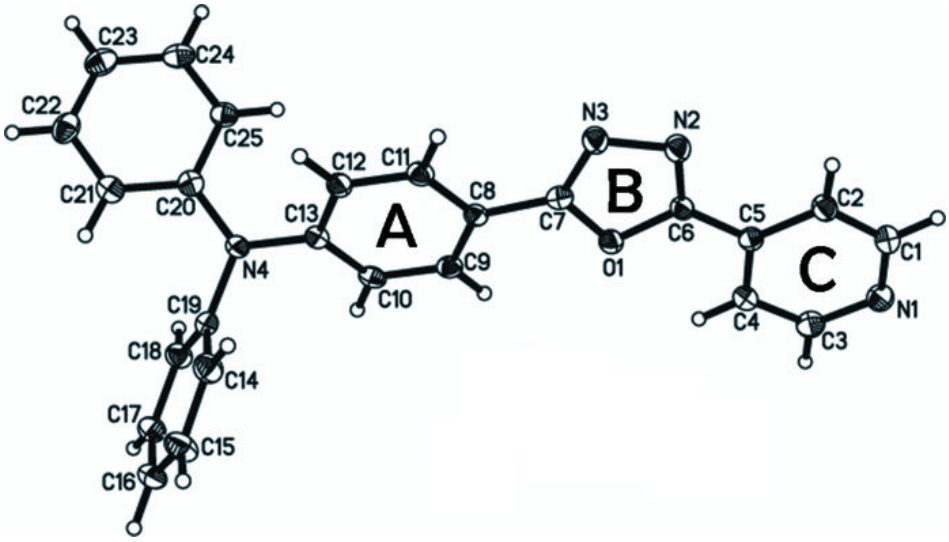
Geometric parameters (Å, °)

C1—N1	1.344 (4)	C13—N4	1.425 (4)
C1—C2	1.384 (4)	C14—C15	1.380 (4)
C1—H1	0.9300	C14—C19	1.388 (4)
C2—C5	1.380 (4)	C14—H14	0.9300
C2—H2	0.9300	C15—C16	1.375 (5)
C3—N1	1.333 (4)	C15—H15	0.9300
C3—C4	1.382 (4)	C16—C17	1.374 (5)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.387 (4)	C17—C18	1.383 (4)
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.452 (4)	C18—C19	1.380 (4)
C6—N2	1.292 (3)	C18—H18	0.9300
C6—O1	1.368 (3)	C19—N4	1.430 (4)
C7—N3	1.296 (4)	C20—C21	1.390 (4)
C7—O1	1.367 (3)	C20—N4	1.399 (4)
C7—C8	1.456 (4)	C20—C25	1.405 (4)
C8—C9	1.387 (4)	C21—C22	1.393 (4)
C8—C11	1.393 (4)	C21—H21	0.9300
C9—C10	1.383 (4)	C22—C23	1.379 (5)
C9—H9	0.9300	C22—H22	0.9300
C10—C13	1.384 (4)	C23—C24	1.370 (5)
C10—H10	0.9300	C23—H23	0.9300
C11—C12	1.381 (4)	C24—C25	1.383 (4)
C11—H11	0.9300	C24—H24	0.9300
C12—C13	1.388 (4)	C25—H25	0.9300
C12—H12	0.9300	N2—N3	1.398 (3)
N1—C1—C2	123.8 (3)	C19—C14—H14	120.0
N1—C1—H1	118.1	C16—C15—C14	120.6 (3)

C2—C1—H1	118.1	C16—C15—H15	119.7
C5—C2—C1	118.8 (3)	C14—C15—H15	119.7
C5—C2—H2	120.6	C17—C16—C15	119.2 (3)
C1—C2—H2	120.6	C17—C16—H16	120.4
N1—C3—C4	124.2 (3)	C15—C16—H16	120.4
N1—C3—H3	117.9	C16—C17—C18	121.2 (3)
C4—C3—H3	117.9	C16—C17—H17	119.4
C3—C4—C5	118.7 (3)	C18—C17—H17	119.4
C3—C4—H4	120.7	C19—C18—C17	119.4 (3)
C5—C4—H4	120.7	C19—C18—H18	120.3
C2—C5—C4	118.3 (3)	C17—C18—H18	120.3
C2—C5—C6	119.8 (3)	C18—C19—C14	119.7 (3)
C4—C5—C6	121.9 (3)	C18—C19—N4	121.3 (3)
N2—C6—O1	112.1 (3)	C14—C19—N4	118.9 (3)
N2—C6—C5	128.1 (3)	C21—C20—N4	121.1 (3)
O1—C6—C5	119.8 (3)	C21—C20—C25	118.0 (3)
N3—C7—O1	112.2 (3)	N4—C20—C25	120.8 (3)
N3—C7—C8	128.5 (3)	C20—C21—C22	120.4 (3)
O1—C7—C8	119.3 (3)	C20—C21—H21	119.8
C9—C8—C11	119.4 (3)	C22—C21—H21	119.8
C9—C8—C7	121.4 (3)	C23—C22—C21	120.9 (3)
C11—C8—C7	119.1 (3)	C23—C22—H22	119.6
C10—C9—C8	120.2 (3)	C21—C22—H22	119.6
C10—C9—H9	119.9	C24—C23—C22	119.0 (3)
C8—C9—H9	119.9	C24—C23—H23	120.5
C9—C10—C13	120.3 (3)	C22—C23—H23	120.5
C9—C10—H10	119.8	C23—C24—C25	121.2 (3)
C13—C10—H10	119.8	C23—C24—H24	119.4
C12—C11—C8	120.3 (3)	C25—C24—H24	119.4
C12—C11—H11	119.9	C24—C25—C20	120.4 (3)
C8—C11—H11	119.9	C24—C25—H25	119.8
C11—C12—C13	120.1 (3)	C20—C25—H25	119.8
C11—C12—H12	120.0	C3—N1—C1	116.3 (3)
C13—C12—H12	120.0	C6—N2—N3	106.8 (2)
C10—C13—C12	119.8 (3)	C7—N3—N2	106.3 (2)
C10—C13—N4	119.6 (3)	C20—N4—C13	121.4 (2)
C12—C13—N4	120.6 (3)	C20—N4—C19	121.8 (2)
C15—C14—C19	119.9 (3)	C13—N4—C19	116.6 (2)
C15—C14—H14	120.0	C7—O1—C6	102.6 (2)
N1—C1—C2—C5	0.8 (5)	N4—C20—C21—C22	176.1 (3)
N1—C3—C4—C5	0.3 (5)	C25—C20—C21—C22	−0.3 (4)
C1—C2—C5—C4	0.2 (5)	C20—C21—C22—C23	−0.2 (5)
C1—C2—C5—C6	−178.3 (3)	C21—C22—C23—C24	1.2 (5)
C3—C4—C5—C2	−0.7 (5)	C22—C23—C24—C25	−1.7 (5)
C3—C4—C5—C6	177.8 (3)	C23—C24—C25—C20	1.2 (5)
C2—C5—C6—N2	−2.4 (5)	C21—C20—C25—C24	−0.2 (4)
C4—C5—C6—N2	179.2 (3)	N4—C20—C25—C24	−176.6 (3)
C2—C5—C6—O1	176.7 (3)	C4—C3—N1—C1	0.7 (5)
C4—C5—C6—O1	−1.7 (4)	C2—C1—N1—C3	−1.2 (5)

N3—C7—C8—C9	−169.3 (3)	O1—C6—N2—N3	0.7 (3)
O1—C7—C8—C9	8.3 (4)	C5—C6—N2—N3	179.8 (3)
N3—C7—C8—C11	8.1 (5)	O1—C7—N3—N2	1.0 (3)
O1—C7—C8—C11	−174.3 (3)	C8—C7—N3—N2	178.8 (3)
C11—C8—C9—C10	−2.2 (4)	C6—N2—N3—C7	−1.0 (3)
C7—C8—C9—C10	175.2 (3)	C21—C20—N4—C13	162.2 (3)
C8—C9—C10—C13	0.3 (4)	C25—C20—N4—C13	−21.5 (4)
C9—C8—C11—C12	2.1 (4)	C21—C20—N4—C19	−12.8 (4)
C7—C8—C11—C12	−175.4 (3)	C25—C20—N4—C19	163.5 (3)
C8—C11—C12—C13	−0.2 (4)	C10—C13—N4—C20	126.7 (3)
C9—C10—C13—C12	1.6 (4)	C12—C13—N4—C20	−52.7 (4)
C9—C10—C13—N4	−177.7 (3)	C10—C13—N4—C19	−58.1 (4)
C11—C12—C13—C10	−1.6 (4)	C12—C13—N4—C19	122.6 (3)
C11—C12—C13—N4	177.7 (3)	C18—C19—N4—C20	−63.3 (4)
C19—C14—C15—C16	1.6 (5)	C14—C19—N4—C20	118.5 (3)
C14—C15—C16—C17	−0.7 (5)	C18—C19—N4—C13	121.5 (3)
C15—C16—C17—C18	−0.8 (5)	C14—C19—N4—C13	−56.7 (4)
C16—C17—C18—C19	1.3 (5)	N3—C7—O1—C6	−0.6 (3)
C17—C18—C19—C14	−0.4 (5)	C8—C7—O1—C6	−178.6 (2)
C17—C18—C19—N4	−178.6 (3)	N2—C6—O1—C7	−0.1 (3)
C15—C14—C19—C18	−1.1 (5)	C5—C6—O1—C7	−179.3 (3)
C15—C14—C19—N4	177.2 (3)		

Fig. 1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C16

Fig. 2