Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,5-Dibenzyl-3-propargyl-1,5-benzodiazepine-2,4-dione

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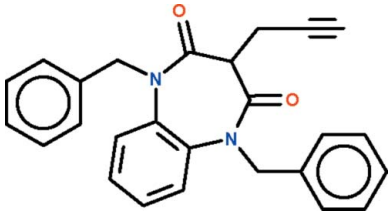
Received 12 November 2009; accepted 15 November 2009

Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.040; wR factor = 0.112; data-to-parameter ratio = 17.1.

The title compound, $C_{26}H_{22}N_2O_2$, features a benzene ring fused with a seven-membered diazepine ring; the latter ring adopts a boat conformation (with the propargylallyl-bearing C atom as the prow and the fused-ring C atoms as the stern). The phenyl ring of one of the two benzyl substituents is disordered over two positions in a 0.812 (11):0.188 (11) ratio.

Related literature

For the crystal structure of the parent compound, benzodiazepin-2,4-dione, see: Négrier *et al.* (2006).



Experimental

Crystal data

$C_{26}H_{22}N_2O_2$
M_r = 394.46
Monoclinic, $P2_1/c$
a = 8.8663 (2) Å
b = 18.6771 (4) Å
c = 12.4665 (3) Å
β = 91.154 (1)°
V = 2063.99 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 193 K
0.70 × 0.50 × 0.30 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: none
29296 measured reflections
4750 independent reflections
3931 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.02
4750 reflections
278 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank Université Mohammed V-Agdal and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2679).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Négrier, Ph., Mondieig, D., Léger, J. M., Benali, B., Lazar, Z., Boucetta, A., Elassyry, A., Lakhrissi, B., Jermoumi, C. & Massoui, M. (2006). *Anal. Sci. X-ray Struct. Anal. Online*, **22**, 175.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2009). E**65**, o3149 [**doi:10.1107/S1600536809048508**]

1,5-Dibenzyl-3-propargyl-1,5-benzodiazepine-2,4-dione

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Experimental

To a solution of the potassium *t*-butoxide (0.24 g, 2.13 mmol) in THF (15 ml) was added 1,5-dibenzyl-1,5-benzodiazepine-2,4-dione (0.50 g, 1.40 mmol) and propargyl bromide (0.20 ml, 1.88 mmol). Stirring was continued for 24 h. The reaction was monitored by thin layer chromatography. The mixture was filtered and the solution evaporated to give colorless crystals.

A somewhat large crystal was used in the diffraction measurements.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 1.00 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C).

One of the phenyl rings is disordered over two positions. This was refined as two rigid hexagons of 1.39 Å sides. The temperature factors of the primed atoms were restrained to those of the unprimed ones. The minor component refined to 0.188 (11).

Figures

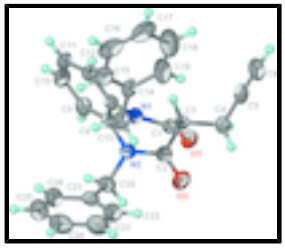


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{26}H_{22}N_2O_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in one of the phenyl rings is not shown.

1,5-Dibenzyl-3-propargyl-1,5-benzodiazepine-2,4-dione

Crystal data

$C_{26}H_{22}N_2O_2$	F_{000} = 832
M_r = 394.46	D_x = 1.269 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9973 reflections
a = 8.8663 (2) Å	θ = 2.5–32.9º
b = 18.6771 (4) Å	μ = 0.08 mm^{-1}
c = 12.4665 (3) Å	T = 193 K
β = 91.154 (1)º	Irregular block, colorless

V = 2063.99 (8) Å^3	0.70 × 0.50 × 0.30 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	3931 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.027
Monochromator: graphite	θ_{max} = 27.5º
T = 193 K	θ_{min} = 2.0º
φ and ω scans	h = −11→11
Absorption correction: None	k = −24→18
29296 measured reflections	l = −16→15
4750 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.112	$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.5557P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
4750 reflections	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
278 parameters	$\Delta\rho_{min}$ = −0.27 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}	Occ. (<1)
O1	0.17022 (9)	0.29934 (4)	0.63891 (7)	0.0310 (2)	
O2	−0.09780 (10)	0.44893 (5)	0.68067 (8)	0.0408 (2)	
N1	0.34007 (10)	0.38740 (5)	0.67524 (7)	0.0250 (2)	
N2	0.12855 (11)	0.50134 (5)	0.71936 (7)	0.0264 (2)	
C1	0.20965 (12)	0.36186 (6)	0.62971 (8)	0.0238 (2)	
C2	0.03474 (13)	0.45816 (6)	0.66023 (9)	0.0268 (2)	
C3	0.11097 (12)	0.41712 (6)	0.57026 (8)	0.0238 (2)	
H3	0.1753	0.4501	0.5277	0.029*	
C4	−0.00697 (13)	0.38106 (6)	0.49721 (9)	0.0285 (2)	
H4A	−0.0646	0.3461	0.5398	0.034*	
H4B	−0.0787	0.4178	0.4701	0.034*	
C5	0.05908 (14)	0.34408 (7)	0.40583 (10)	0.0334 (3)	
C6	0.11070 (17)	0.31415 (8)	0.33138 (12)	0.0461 (3)	
H6	0.1521	0.2901	0.2716	0.055*	
C7	0.38435 (13)	0.46069 (6)	0.67074 (8)	0.0249 (2)	
C8	0.28132 (13)	0.51554 (6)	0.69185 (8)	0.0255 (2)	

C9	0.33036 (15)	0.58677 (7)	0.68953 (10)	0.0332 (3)	
H9	0.2605	0.6244	0.7011	0.040*	
C10	0.47975 (16)	0.60272 (7)	0.67056 (10)	0.0384 (3)	
H10	0.5122	0.6512	0.6700	0.046*	
C11	0.58233 (15)	0.54818 (7)	0.65236 (10)	0.0369 (3)	
H11	0.6853	0.5593	0.6410	0.044*	
C12	0.53473 (14)	0.47752 (7)	0.65072 (9)	0.0314 (3)	
H12	0.6046	0.4404	0.6359	0.038*	
C13	0.43658 (14)	0.33760 (7)	0.73776 (10)	0.0320 (3)	
H13A	0.4796	0.3649	0.7991	0.038*	0.188 (11)
H13B	0.3695	0.3008	0.7681	0.038*	0.188 (11)
H13C	0.3715	0.3028	0.7748	0.038*	0.812 (11)
H13D	0.4930	0.3650	0.7934	0.038*	0.812 (11)
C14'	0.5525 (9)	0.3026 (8)	0.6915 (10)	0.0290 (5)	0.188 (11)
C15'	0.6972 (11)	0.3031 (7)	0.7365 (9)	0.0426 (6)	0.188 (11)
H15'	0.7173	0.3290	0.8008	0.051*	0.188 (11)
C16'	0.8126 (8)	0.2659 (7)	0.6873 (11)	0.0480 (10)	0.188 (11)
H16'	0.9115	0.2663	0.7180	0.058*	0.188 (11)
C17'	0.7832 (12)	0.2281 (6)	0.5931 (12)	0.0511 (8)	0.188 (11)
H17'	0.8621	0.2026	0.5595	0.061*	0.188 (11)
C18'	0.6385 (14)	0.2275 (8)	0.5482 (12)	0.0728 (9)	0.188 (11)
H18'	0.6184	0.2017	0.4838	0.087*	0.188 (11)
C19'	0.5231 (10)	0.2648 (9)	0.5974 (11)	0.0567 (7)	0.188 (11)
H19'	0.4242	0.2644	0.5667	0.068*	0.188 (11)
C14	0.5505 (2)	0.29604 (17)	0.6685 (3)	0.0290 (5)	0.812 (11)
C15	0.6962 (2)	0.28451 (19)	0.7075 (3)	0.0426 (6)	0.812 (11)
H15	0.7261	0.3039	0.7751	0.051*	0.812 (11)
C16	0.7990 (2)	0.2450 (2)	0.6492 (4)	0.0480 (10)	0.812 (11)
H16	0.8979	0.2373	0.6775	0.058*	0.812 (11)
C17	0.7587 (3)	0.21739 (14)	0.5519 (4)	0.0511 (8)	0.812 (11)
H17	0.8288	0.1903	0.5121	0.061*	0.812 (11)
C18	0.6154 (3)	0.22919 (19)	0.5119 (4)	0.0728 (9)	0.812 (11)
H18	0.5870	0.2105	0.4436	0.087*	0.812 (11)
C19	0.5119 (3)	0.2679 (2)	0.5699 (3)	0.0567 (7)	0.812 (11)
H19	0.4131	0.2752	0.5412	0.068*	0.812 (11)
C20	0.07850 (14)	0.52656 (7)	0.82584 (9)	0.0313 (3)	
H20A	−0.0327	0.5235	0.8295	0.038*	
H20B	0.1083	0.5772	0.8365	0.038*	
C21	0.15023 (14)	0.48060 (7)	0.91273 (9)	0.0305 (3)	
C22	0.11027 (17)	0.40885 (7)	0.92212 (10)	0.0396 (3)	
H22	0.0354	0.3893	0.8751	0.047*	
C23	0.17857 (19)	0.36561 (8)	0.99950 (12)	0.0482 (4)	
H23	0.1511	0.3166	1.0048	0.058*	
C24	0.28666 (18)	0.39393 (9)	1.06888 (11)	0.0505 (4)	
H24	0.3327	0.3645	1.1224	0.061*	
C25	0.32761 (19)	0.46476 (10)	1.06047 (12)	0.0522 (4)	
H25	0.4021	0.4841	1.1080	0.063*	
C26	0.25989 (16)	0.50798 (8)	0.98237 (11)	0.0415 (3)	
H26	0.2890	0.5568	0.9767	0.050*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0302 (4)	0.0243 (4)	0.0384 (4)	−0.0013 (3)	−0.0020 (3)	0.0049 (3)
O2	0.0226 (4)	0.0483 (6)	0.0516 (6)	0.0013 (4)	0.0039 (4)	−0.0121 (4)
N1	0.0235 (5)	0.0243 (5)	0.0272 (4)	0.0033 (4)	−0.0028 (4)	0.0014 (3)
N2	0.0249 (5)	0.0275 (5)	0.0269 (5)	0.0028 (4)	0.0014 (4)	−0.0024 (4)
C1	0.0232 (5)	0.0249 (5)	0.0233 (5)	0.0015 (4)	0.0013 (4)	0.0008 (4)
C2	0.0236 (6)	0.0262 (5)	0.0306 (5)	0.0040 (4)	−0.0011 (4)	0.0010 (4)
C3	0.0239 (5)	0.0228 (5)	0.0246 (5)	0.0006 (4)	−0.0020 (4)	0.0015 (4)
C4	0.0272 (6)	0.0279 (6)	0.0302 (5)	−0.0007 (4)	−0.0063 (4)	0.0013 (4)
C5	0.0338 (6)	0.0305 (6)	0.0355 (6)	−0.0041 (5)	−0.0096 (5)	−0.0020 (5)
C6	0.0457 (8)	0.0493 (8)	0.0430 (7)	−0.0003 (7)	−0.0068 (6)	−0.0156 (6)
C7	0.0257 (5)	0.0264 (5)	0.0225 (5)	−0.0006 (4)	−0.0021 (4)	−0.0012 (4)
C8	0.0251 (6)	0.0279 (5)	0.0234 (5)	−0.0006 (4)	−0.0018 (4)	−0.0010 (4)
C9	0.0369 (7)	0.0268 (6)	0.0358 (6)	0.0002 (5)	−0.0030 (5)	−0.0029 (5)
C10	0.0424 (7)	0.0309 (6)	0.0417 (7)	−0.0111 (5)	−0.0010 (6)	−0.0012 (5)
C11	0.0301 (6)	0.0435 (7)	0.0371 (6)	−0.0114 (5)	0.0023 (5)	−0.0031 (5)
C12	0.0260 (6)	0.0363 (6)	0.0318 (6)	−0.0005 (5)	0.0013 (4)	−0.0035 (5)
C13	0.0311 (6)	0.0324 (6)	0.0322 (6)	0.0037 (5)	−0.0096 (5)	0.0045 (5)
C14'	0.0251 (6)	0.0232 (8)	0.0384 (13)	0.0018 (5)	−0.0039 (7)	0.0042 (8)
C15'	0.0285 (7)	0.0577 (15)	0.0414 (14)	0.0039 (9)	−0.0049 (8)	0.0094 (11)
C16'	0.0246 (8)	0.0538 (16)	0.066 (2)	0.0098 (9)	0.0024 (10)	0.0223 (16)
C17'	0.0350 (11)	0.0326 (9)	0.086 (2)	0.0053 (8)	0.0170 (12)	−0.0031 (11)
C18'	0.0433 (12)	0.0895 (15)	0.086 (2)	0.0116 (11)	−0.0022 (13)	−0.0534 (17)
C19'	0.0300 (8)	0.0751 (12)	0.0647 (18)	0.0138 (8)	−0.0097 (9)	−0.0338 (14)
C14	0.0251 (6)	0.0232 (8)	0.0384 (13)	0.0018 (5)	−0.0039 (7)	0.0042 (8)
C15	0.0285 (7)	0.0577 (15)	0.0414 (14)	0.0039 (9)	−0.0049 (8)	0.0094 (11)
C16	0.0246 (8)	0.0538 (16)	0.066 (2)	0.0098 (9)	0.0024 (10)	0.0223 (16)
C17	0.0350 (11)	0.0326 (9)	0.086 (2)	0.0053 (8)	0.0170 (12)	−0.0031 (11)
C18	0.0433 (12)	0.0895 (15)	0.086 (2)	0.0116 (11)	−0.0022 (13)	−0.0534 (17)
C19	0.0300 (8)	0.0751 (12)	0.0647 (18)	0.0138 (8)	−0.0097 (9)	−0.0338 (14)
C20	0.0313 (6)	0.0314 (6)	0.0313 (6)	0.0061 (5)	0.0046 (5)	−0.0057 (5)
C21	0.0294 (6)	0.0350 (6)	0.0273 (5)	0.0027 (5)	0.0070 (4)	−0.0035 (4)
C22	0.0442 (8)	0.0391 (7)	0.0355 (6)	−0.0043 (6)	0.0008 (5)	−0.0016 (5)
C23	0.0620 (10)	0.0395 (7)	0.0433 (7)	0.0013 (7)	0.0074 (7)	0.0067 (6)
C24	0.0524 (9)	0.0622 (10)	0.0369 (7)	0.0101 (8)	0.0009 (6)	0.0118 (7)
C25	0.0473 (9)	0.0694 (10)	0.0394 (7)	−0.0062 (8)	−0.0092 (6)	0.0018 (7)
C26	0.0430 (8)	0.0436 (7)	0.0378 (7)	−0.0062 (6)	−0.0010 (6)	−0.0024 (6)

Geometric parameters (Å, °)

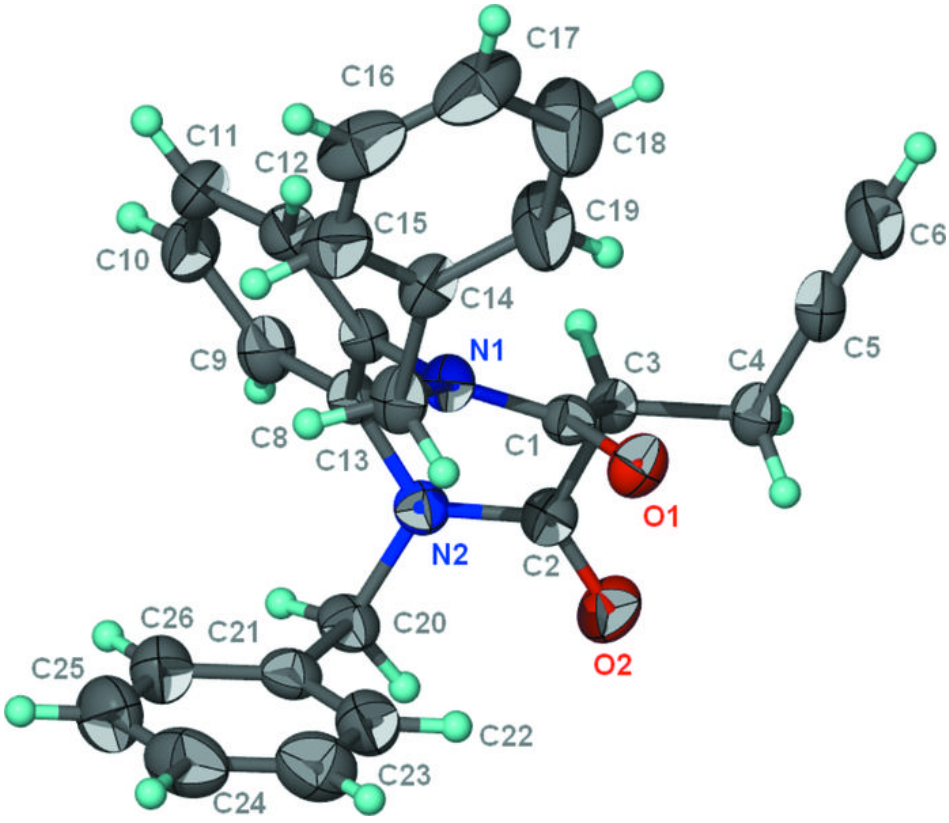
O1—C1	1.2248 (13)	C15'—C16'	1.3900
O2—C2	1.2197 (15)	C15'—H15'	0.9500
N1—C1	1.3640 (14)	C16'—C17'	1.3900
N1—C7	1.4254 (14)	C16'—H16'	0.9500
N1—C13	1.4758 (14)	C17'—C18'	1.3900
N2—C2	1.3641 (15)	C17'—H17'	0.9500

N2—C8	1.4288 (15)	C18'—C19'	1.3900
N2—C20	1.4847 (14)	C18'—H18'	0.9500
C1—C3	1.5342 (14)	C19'—H19'	0.9500
C2—C3	1.5274 (15)	C14—C19	1.373 (2)
C3—C4	1.5291 (15)	C14—C15	1.388 (2)
C3—H3	1.0000	C15—C16	1.389 (3)
C4—C5	1.4645 (18)	C15—H15	0.9500
C4—H4A	0.9900	C16—C17	1.359 (3)
C4—H4B	0.9900	C16—H16	0.9500
C5—C6	1.1833 (19)	C17—C18	1.373 (3)
C6—H6	0.9500	C17—H17	0.9500
C7—C12	1.3972 (17)	C18—C19	1.384 (3)
C7—C8	1.4010 (16)	C18—H18	0.9500
C8—C9	1.4001 (17)	C19—H19	0.9500
C9—C10	1.3826 (19)	C20—C21	1.5122 (17)
C9—H9	0.9500	C20—H20A	0.9900
C10—C11	1.387 (2)	C20—H20B	0.9900
C10—H10	0.9500	C21—C26	1.3880 (18)
C11—C12	1.3856 (18)	C21—C22	1.3918 (18)
C11—H11	0.9500	C22—C23	1.388 (2)
C12—H12	0.9500	C22—H22	0.9500
C13—C14'	1.356 (8)	C23—C24	1.383 (2)
C13—C14	1.550 (3)	C23—H23	0.9500
C13—H13A	0.9900	C24—C25	1.376 (2)
C13—H13B	0.9900	C24—H24	0.9500
C13—H13C	0.9900	C25—C26	1.392 (2)
C13—H13D	0.9900	C25—H25	0.9500
C14'—C15'	1.3900	C26—H26	0.9500
C14'—C19'	1.3900		
C1—N1—C7	123.46 (9)	C13—C14'—C15'	121.8 (7)
C1—N1—C13	118.49 (9)	C13—C14'—C19'	118.2 (7)
C7—N1—C13	117.96 (9)	C15'—C14'—C19'	120.0
C2—N2—C8	123.41 (9)	C14'—C15'—C16'	120.0
C2—N2—C20	118.73 (10)	C14'—C15'—H15'	120.0
C8—N2—C20	117.23 (9)	C16'—C15'—H15'	120.0
O1—C1—N1	122.39 (10)	C15'—C16'—C17'	120.0
O1—C1—C3	121.70 (10)	C15'—C16'—H16'	120.0
N1—C1—C3	115.86 (9)	C17'—C16'—H16'	120.0
O2—C2—N2	123.38 (11)	C18'—C17'—C16'	120.0
O2—C2—C3	121.66 (10)	C18'—C17'—H17'	120.0
N2—C2—C3	114.81 (10)	C16'—C17'—H17'	120.0
C2—C3—C4	110.55 (9)	C19'—C18'—C17'	120.0
C2—C3—C1	103.86 (8)	C19'—C18'—H18'	120.0
C4—C3—C1	111.59 (9)	C17'—C18'—H18'	120.0
C2—C3—H3	110.2	C18'—C19'—C14'	120.0
C4—C3—H3	110.2	C18'—C19'—H19'	120.0
C1—C3—H3	110.2	C14'—C19'—H19'	120.0
C5—C4—C3	113.06 (10)	C19—C14—C15	117.86 (16)
C5—C4—H4A	109.0	C19—C14—C13	122.45 (17)

C3—C4—H4A	109.0	C15—C14—C13	119.66 (16)
C5—C4—H4B	109.0	C14—C15—C16	120.98 (18)
C3—C4—H4B	109.0	C14—C15—H15	119.5
H4A—C4—H4B	107.8	C16—C15—H15	119.5
C6—C5—C4	179.17 (14)	C17—C16—C15	120.36 (17)
C5—C6—H6	180.0	C17—C16—H16	119.8
C12—C7—C8	119.81 (10)	C15—C16—H16	119.8
C12—C7—N1	119.19 (10)	C16—C17—C18	119.18 (18)
C8—C7—N1	120.91 (10)	C16—C17—H17	120.4
C9—C8—C7	119.14 (11)	C18—C17—H17	120.4
C9—C8—N2	118.53 (10)	C17—C18—C19	120.8 (2)
C7—C8—N2	122.29 (10)	C17—C18—H18	119.6
C10—C9—C8	120.48 (12)	C19—C18—H18	119.6
C10—C9—H9	119.8	C14—C19—C18	120.79 (18)
C8—C9—H9	119.8	C14—C19—H19	119.6
C9—C10—C11	120.21 (12)	C18—C19—H19	119.6
C9—C10—H10	119.9	N2—C20—C21	109.35 (9)
C11—C10—H10	119.9	N2—C20—H20A	109.8
C12—C11—C10	120.08 (12)	C21—C20—H20A	109.8
C12—C11—H11	120.0	N2—C20—H20B	109.8
C10—C11—H11	120.0	C21—C20—H20B	109.8
C11—C12—C7	120.21 (12)	H20A—C20—H20B	108.3
C11—C12—H12	119.9	C26—C21—C22	118.58 (12)
C7—C12—H12	119.9	C26—C21—C20	121.21 (12)
C14'—C13—N1	121.1 (6)	C22—C21—C20	120.18 (11)
N1—C13—C14	113.51 (14)	C23—C22—C21	120.70 (13)
C14'—C13—H13A	107.1	C23—C22—H22	119.7
N1—C13—H13A	107.1	C21—C22—H22	119.7
C14—C13—H13A	116.3	C24—C23—C22	119.96 (14)
C14'—C13—H13B	107.1	C24—C23—H23	120.0
N1—C13—H13B	107.1	C22—C23—H23	120.0
C14—C13—H13B	105.6	C25—C24—C23	120.03 (14)
H13A—C13—H13B	106.8	C25—C24—H24	120.0
C14'—C13—H13C	109.6	C23—C24—H24	120.0
N1—C13—H13C	108.9	C24—C25—C26	120.00 (14)
C14—C13—H13C	108.9	C24—C25—H25	120.0
H13A—C13—H13C	101.4	C26—C25—H25	120.0
N1—C13—H13D	108.9	C21—C26—C25	120.73 (14)
C14—C13—H13D	108.9	C21—C26—H26	119.6
H13C—C13—H13D	107.7	C25—C26—H26	119.6
C7—N1—C1—O1	−176.41 (10)	C1—N1—C13—C14	87.11 (17)
C13—N1—C1—O1	−0.01 (16)	C7—N1—C13—C14	−96.30 (16)
C7—N1—C1—C3	0.87 (15)	N1—C13—C14'—C15'	128.9 (7)
C13—N1—C1—C3	177.26 (9)	C14—C13—C14'—C15'	169 (5)
C8—N2—C2—O2	−176.15 (11)	N1—C13—C14'—C19'	−51.8 (9)
C20—N2—C2—O2	13.17 (17)	C14—C13—C14'—C19'	−11 (4)
C8—N2—C2—C3	8.29 (15)	C13—C14'—C15'—C16'	179.3 (12)
C20—N2—C2—C3	−162.38 (9)	C19'—C14'—C15'—C16'	0.0
O2—C2—C3—C4	14.32 (15)	C14'—C15'—C16'—C17'	0.0

N2—C2—C3—C4	−170.04 (9)	C15'—C16'—C17'—C18'	0.0
O2—C2—C3—C1	−105.49 (12)	C16'—C17'—C18'—C19'	0.0
N2—C2—C3—C1	70.14 (11)	C17'—C18'—C19'—C14'	0.0
O1—C1—C3—C2	100.64 (12)	C13—C14'—C19'—C18'	−179.3 (12)
N1—C1—C3—C2	−76.66 (11)	C15'—C14'—C19'—C18'	0.0
O1—C1—C3—C4	−18.46 (15)	C14'—C13—C14—C19	175 (5)
N1—C1—C3—C4	164.24 (9)	N1—C13—C14—C19	−41.8 (3)
C2—C3—C4—C5	176.83 (9)	C14'—C13—C14—C15	−3(4)
C1—C3—C4—C5	−68.12 (12)	N1—C13—C14—C15	140.1 (2)
C1—N1—C7—C12	−137.80 (11)	C19—C14—C15—C16	−0.8 (3)
C13—N1—C7—C12	45.79 (14)	C13—C14—C15—C16	177.4 (2)
C1—N1—C7—C8	45.72 (15)	C14—C15—C16—C17	0.6 (3)
C13—N1—C7—C8	−130.69 (11)	C15—C16—C17—C18	0.2 (3)
C12—C7—C8—C9	1.77 (16)	C16—C17—C18—C19	−0.8 (4)
N1—C7—C8—C9	178.23 (10)	C15—C14—C19—C18	0.2 (3)
C12—C7—C8—N2	−176.05 (10)	C13—C14—C19—C18	−177.9 (3)
N1—C7—C8—N2	0.41 (15)	C17—C18—C19—C14	0.6 (4)
C2—N2—C8—C9	130.25 (12)	C2—N2—C20—C21	99.41 (12)
C20—N2—C8—C9	−58.95 (14)	C8—N2—C20—C21	−71.84 (13)
C2—N2—C8—C7	−51.91 (15)	N2—C20—C21—C26	110.77 (13)
C20—N2—C8—C7	118.89 (11)	N2—C20—C21—C22	−67.23 (15)
C7—C8—C9—C10	−2.35 (17)	C26—C21—C22—C23	0.0 (2)
N2—C8—C9—C10	175.55 (11)	C20—C21—C22—C23	178.08 (12)
C8—C9—C10—C11	0.75 (19)	C21—C22—C23—C24	0.6 (2)
C9—C10—C11—C12	1.46 (19)	C22—C23—C24—C25	−0.7 (2)
C10—C11—C12—C7	−2.03 (19)	C23—C24—C25—C26	0.2 (2)
C8—C7—C12—C11	0.40 (17)	C22—C21—C26—C25	−0.5 (2)
N1—C7—C12—C11	−176.12 (10)	C20—C21—C26—C25	−178.52 (13)
C1—N1—C13—C14'	93.9 (7)	C24—C25—C26—C21	0.4 (2)
C7—N1—C13—C14'	−89.5 (7)		

Fig. 1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