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3,5-Dimethyl-1-(triphenylmethyl)-1*H*-pyrazole

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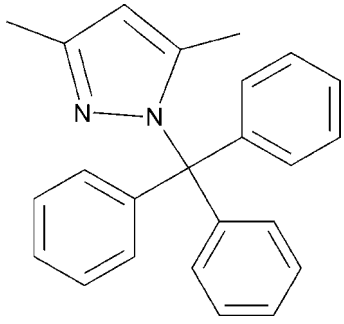
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.095; data-to-parameter ratio = 15.6.

In the title compound, $C_{24}H_{22}N_2$, the bond distances and angles are typical. The central C atom exhibits a distorted tetrahedral geometry; the angles range from 106.17 (8) to 113.01 (9)°. The torsion angles N—C—C(*ipso*)—C(*ortho*) involving the phenyl rings are very different, at 5.20 (14), 46.68 (12) and 69.65 (12)°.

Related literature

For related literature, see: Allen (2002); Brown & Kee (1993); Elguero (1996); Esquius *et al.* (2000).



Experimental

Crystal data

$C_{24}H_{22}N_2$
M_r = 338.44
Monoclinic, $P2_1/c$
a = 9.5264 (5) Å
b = 8.6992 (4) Å
c = 21.9714 (11) Å
β = 93.9610 (10)°
V = 1816.47 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 100 (2) K
0.41 × 0.27 × 0.19 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.971, T_{max} = 0.986
14683 measured reflections
3708 independent reflections
3141 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
S = 1.03
3708 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected bond angles (°).

N1—C6—C7	110.07 (8)	N1—C6—C19	109.44 (8)
N1—C6—C13	106.17 (8)	C7—C6—C19	107.23 (8)
C7—C6—C13	113.01 (9)	C13—C6—C19	110.91 (8)

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *publCIF* (Westrip, 2007) and *modiCIFer* (Guzei, 2007).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2051).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Brown, T. L. & Kee, K. J. (1993). *Coord. Chem. Rev.* **128**, 89–116.
Bruker (2003). *SADABS* (Version 2.05), *SAINT* (Version 6.22), *SHELXTL* (Version 6.10), and *SMART* (Version 5.622). Bruker AXS Inc., Madison, Wisconsin, USA.
Elguero, J. (1996). *Comprehensive Heteroyclic Chemistry II: Pyrazoles*, Vol. 3, edited by A. R. Katrizky, C. W. Rees & E. F. V. Scriven, pp. 1–75. Oxford: Pergamon Press.
Esquius, G., Pons, J., Yáñez, R., Ros, J., Solans, X. & Font-Bardía, M. (2000). *J. Organomet. Chem.* **605**, 226–233.
Guzei, I. A. (2007). *modiCIFer*. University of Wisconsin–Madison, USA.
Westrip, S. P. (2007). *publCIF*. In preparation.

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supplementary materials

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3,5-Dimethyl-1-(triphenylmethyl)-1*H*-pyrazole

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Comment

Water-soluble substituted pyrazoles constitute an important family of heterocyclic compounds that have found use in drug development and in catalysis (Elguero *et al.* 1996, Brown *et al.*, 1993). In attempts to prepare water soluble palladium and platinum complexes with potential anti-cancer properties, we set out to prepare 4-alkylaminopyrazoles using a route reported by Esquius *et al.* (2000). The route involves protection of the position 1 of the 3,5-dimethylpyrazole, followed by aminoalkylation of the position 4. This offers a more efficient route to making water soluble 4-alkylaminopyrazoles (Esquius *et al.* 2000). When we used this route with a trityl group to protect the position 1 of the pyrazole, we could not alkylate position 4 of the pyrazole efficiently and isolated compound (**I**) instead.

Within (I) the bond distances and angles are typical. Carbon atom C6 exhibits a distorted tetrahedral geometry with the average *X*—C6—C angles being 109 (2)°. The six *X*—C6—C angles range from 106.17 (8)° to 113.01 (9)°. The torsion angles N—C—C(*ipso*)-C(*ortho*) involving the phenyl rings are very different at 5.20 (14), 46.68 (12), and 69.65 (12)°. A quality-restrictive search (*R*-factor <0.05, not disordered, no errors, and no powder structures) of the Cambridge Structural Database (Version 5.28, January 2007 update, Allen, 2002) for organic compounds with N-CPh_3 fragments returned 34 hits and revealed that the N—C—C(*ipso*)-C(*ortho*) angles vary to a large extent but are usually different at 13 (9), 36 (10), and 73 (13)°. The trend is in agreement with that of the corresponding parameters in (**I**).

Experimental

A solution of triphenylchloromethane (2.9 g, 10.4 mmol) in toluene (20 ml) was added to a solution of 3,5-dimethylpyrazole (1.0 g, 10.4 mmol) in toluene (20 ml). Triethylammine (2 ml) was added and the solution stirred at 80° C for 15 h. The resultant $Et_3NH^+Cl^-$ salt was removed by filtration and the solution was evaporated to dryness. A brown solid was obtained. The product was purified by chromatography using silica gel and CH_2Cl_2:hexane (5:1) as eluent. Compound (I) crystallized upon slow evaporation of the solvent to give X-ray quality crystals. Yield = 2.57 g (73%). ^{1}H NMR ($CDCl_3$): δ 7.45, 7.14 (15 H, $(C_6H_5)_3$); 6.03 (s, 1H, 4-pz); 2.23 (s, 3H, 5-Me); 1.46 (s, 3H, 3-Me). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 146.0 (C (5-pz)); 144.1 (phenyl); 142.0 (C(3-pz)); 128.0, 127.5 (phenyl); 127.3 (phenyl); 108.1 (C (4-pz)); 82.0 (C ($C(Ph)_3$)); 15.2 (C(CH_3, 5-pz)); 14.6 (C(CH_3, 3-pz)). IR (Nujol): 1701 cm^{-1}($\upsilon_{C=C,pz}$); 1571 cm^{-1} ($\upsilon_{C=N}$).

Refinement

Although all the hydrogen atoms were discernible in the difference Fourier map, they were placed in idealized locations and refined as riding with appropriate thermal displacement coefficients U_{iso}(H) = 1.2 or 1.5 (methyl H atoms) times U_{eq} of the parent atom. The C—H distances were set to 0.98 Å for the hydrogen atoms attached to methyl-carbon atoms C1 and C5 and 0.95 Å for all other hydrogen atoms.

Figures

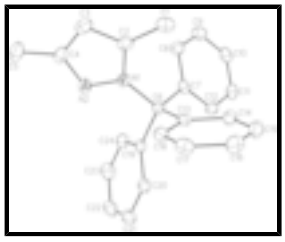


Fig. 1. Molecular structure of (I). The thermal ellipsoids are shown at 50% probability level. All hydrogen atoms were omitted for clarity.

3,5-Dimethyl-1-(triphenylmethyl)-1*H*-pyrazole

Crystal data

$C_{24}H_{22}N_2$	F_{000} = 720
M_r = 338.44	D_x = 1.238 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7180 reflections
a = 9.5264 (5) Å	θ = 2.1–26.4º
b = 8.6992 (4) Å	μ = 0.07 mm^{-1}
c = 21.9714 (11) Å	T = 100 (2) K
β = 93.9610 (10)º	Block, colorless
V = 1816.47 (16) Å^3	0.41 × 0.27 × 0.19 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	3708 independent reflections
Radiation source: fine-focus sealed tube	3141 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 100(2) K	θ_{max} = 26.4º
0.30° ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	h = −11→11
T_{min} = 0.971, T_{max} = 0.986	k = −10→10
14683 measured reflections	l = −27→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.035	H-atom parameters constrained
$wR(F^2)$ = 0.095	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.4396P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001

3708 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
86 constraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	0.19656 (9)	0.32354 (10)	0.32906 (4)	0.0180 (2)
N2	0.31711 (9)	0.23745 (11)	0.33155 (4)	0.0208 (2)
C1	0.01024 (13)	0.42816 (15)	0.25096 (5)	0.0284 (3)
H1A	0.0001	0.4333	0.2063	0.043*
H1B	0.0164	0.5325	0.2677	0.043*
H1C	−0.0715	0.3756	0.2660	0.043*
C2	0.14076 (12)	0.34152 (13)	0.27048 (5)	0.0217 (2)
C3	0.22915 (13)	0.26332 (14)	0.23435 (5)	0.0252 (3)
H3	0.2197	0.2537	0.1912	0.030*
C4	0.33584 (12)	0.20082 (13)	0.27390 (5)	0.0236 (3)
C5	0.45955 (14)	0.10514 (16)	0.25862 (7)	0.0344 (3)
H5A	0.4290	0.0280	0.2280	0.052*
H5B	0.4992	0.0535	0.2955	0.052*
H5C	0.5312	0.1714	0.2423	0.052*
C6	0.14571 (11)	0.39237 (12)	0.38588 (5)	0.0171 (2)
C7	0.18242 (11)	0.56500 (12)	0.38913 (5)	0.0179 (2)
C8	0.24280 (12)	0.64229 (13)	0.34215 (5)	0.0224 (2)
H8	0.2611	0.5888	0.3058	0.027*
C9	0.27665 (12)	0.79768 (14)	0.34788 (6)	0.0258 (3)
H9	0.3174	0.8491	0.3153	0.031*
C10	0.25182 (12)	0.87807 (13)	0.40039 (6)	0.0242 (3)
H10	0.2743	0.9842	0.4039	0.029*
C11	0.19341 (12)	0.80087 (13)	0.44779 (6)	0.0231 (3)
H11	0.1763	0.8544	0.4842	0.028*
C12	0.15986 (11)	0.64602 (13)	0.44236 (5)	0.0202 (2)
H12	0.1209	0.5944	0.4754	0.024*
C13	−0.01407 (11)	0.36151 (12)	0.38356 (5)	0.0169 (2)

C14	−0.11368 (11)	0.47309 (13)	0.39443 (5)	0.0200 (2)
H14	−0.0840	0.5746	0.4048	0.024*
C15	−0.25684 (12)	0.43740 (14)	0.39027 (5)	0.0238 (3)
H15	−0.3236	0.5145	0.3984	0.029*
C16	−0.30255 (12)	0.29088 (14)	0.37438 (5)	0.0248 (3)
H16	−0.4001	0.2672	0.3713	0.030*
C17	−0.20363 (12)	0.17872 (13)	0.36297 (5)	0.0233 (3)
H17	−0.2338	0.0781	0.3515	0.028*
C18	−0.06131 (12)	0.21310 (13)	0.36831 (5)	0.0202 (2)
H18	0.0053	0.1347	0.3615	0.024*
C19	0.22179 (11)	0.31466 (12)	0.44228 (5)	0.0177 (2)
C20	0.15200 (12)	0.22381 (12)	0.48246 (5)	0.0197 (2)
H20	0.0540	0.2055	0.4750	0.024*
C21	0.22369 (13)	0.15898 (13)	0.53369 (5)	0.0251 (3)
H21	0.1740	0.0980	0.5609	0.030*
C22	0.36624 (14)	0.18284 (14)	0.54502 (6)	0.0291 (3)
H22	0.4156	0.1359	0.5792	0.035*
C23	0.43700 (13)	0.27640 (15)	0.50588 (6)	0.0286 (3)
H23	0.5349	0.2948	0.5137	0.034*
C24	0.36525 (12)	0.34268 (13)	0.45559 (5)	0.0230 (3)
H24	0.4142	0.4082	0.4297	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0187 (5)	0.0169 (5)	0.0186 (5)	0.0002 (4)	0.0037 (4)	−0.0016 (4)
N2	0.0178 (5)	0.0179 (5)	0.0275 (5)	0.0001 (4)	0.0063 (4)	−0.0023 (4)
C1	0.0327 (7)	0.0326 (7)	0.0194 (6)	0.0023 (5)	−0.0014 (5)	0.0034 (5)
C2	0.0268 (6)	0.0193 (6)	0.0192 (6)	−0.0044 (5)	0.0033 (4)	−0.0002 (4)
C3	0.0315 (6)	0.0239 (6)	0.0210 (6)	−0.0073 (5)	0.0075 (5)	−0.0030 (5)
C4	0.0240 (6)	0.0201 (6)	0.0281 (6)	−0.0047 (5)	0.0103 (5)	−0.0044 (5)
C5	0.0331 (7)	0.0316 (7)	0.0407 (8)	0.0005 (6)	0.0171 (6)	−0.0078 (6)
C6	0.0181 (5)	0.0168 (5)	0.0168 (5)	0.0001 (4)	0.0038 (4)	−0.0012 (4)
C7	0.0143 (5)	0.0174 (5)	0.0220 (6)	0.0007 (4)	0.0000 (4)	0.0002 (4)
C8	0.0234 (6)	0.0217 (6)	0.0225 (6)	−0.0015 (4)	0.0049 (4)	−0.0006 (4)
C9	0.0254 (6)	0.0229 (6)	0.0296 (7)	−0.0036 (5)	0.0053 (5)	0.0046 (5)
C10	0.0207 (6)	0.0157 (5)	0.0358 (7)	−0.0008 (4)	−0.0007 (5)	−0.0003 (5)
C11	0.0217 (6)	0.0204 (6)	0.0270 (6)	0.0007 (4)	0.0009 (5)	−0.0051 (5)
C12	0.0190 (5)	0.0207 (6)	0.0211 (6)	−0.0003 (4)	0.0026 (4)	−0.0001 (4)
C13	0.0181 (5)	0.0190 (5)	0.0134 (5)	−0.0005 (4)	0.0008 (4)	0.0018 (4)
C14	0.0214 (6)	0.0198 (5)	0.0187 (5)	−0.0002 (4)	0.0014 (4)	−0.0008 (4)
C15	0.0203 (6)	0.0277 (6)	0.0237 (6)	0.0043 (5)	0.0023 (4)	−0.0011 (5)
C16	0.0176 (5)	0.0313 (7)	0.0254 (6)	−0.0030 (5)	0.0003 (4)	0.0015 (5)
C17	0.0242 (6)	0.0217 (6)	0.0234 (6)	−0.0047 (5)	−0.0015 (5)	0.0016 (5)
C18	0.0217 (6)	0.0189 (5)	0.0199 (6)	0.0012 (4)	0.0009 (4)	0.0017 (4)
C19	0.0197 (5)	0.0153 (5)	0.0180 (5)	0.0027 (4)	0.0012 (4)	−0.0031 (4)
C20	0.0220 (6)	0.0165 (5)	0.0208 (6)	0.0004 (4)	0.0021 (4)	−0.0029 (4)
C21	0.0340 (7)	0.0193 (6)	0.0219 (6)	0.0012 (5)	0.0011 (5)	−0.0005 (4)

C22	0.0355 (7)	0.0264 (6)	0.0241 (6)	0.0073 (5)	−0.0070 (5)	0.0009 (5)
C23	0.0220 (6)	0.0305 (7)	0.0323 (7)	0.0029 (5)	−0.0050 (5)	−0.0041 (5)
C24	0.0213 (6)	0.0227 (6)	0.0252 (6)	−0.0004 (5)	0.0020 (5)	−0.0011 (5)

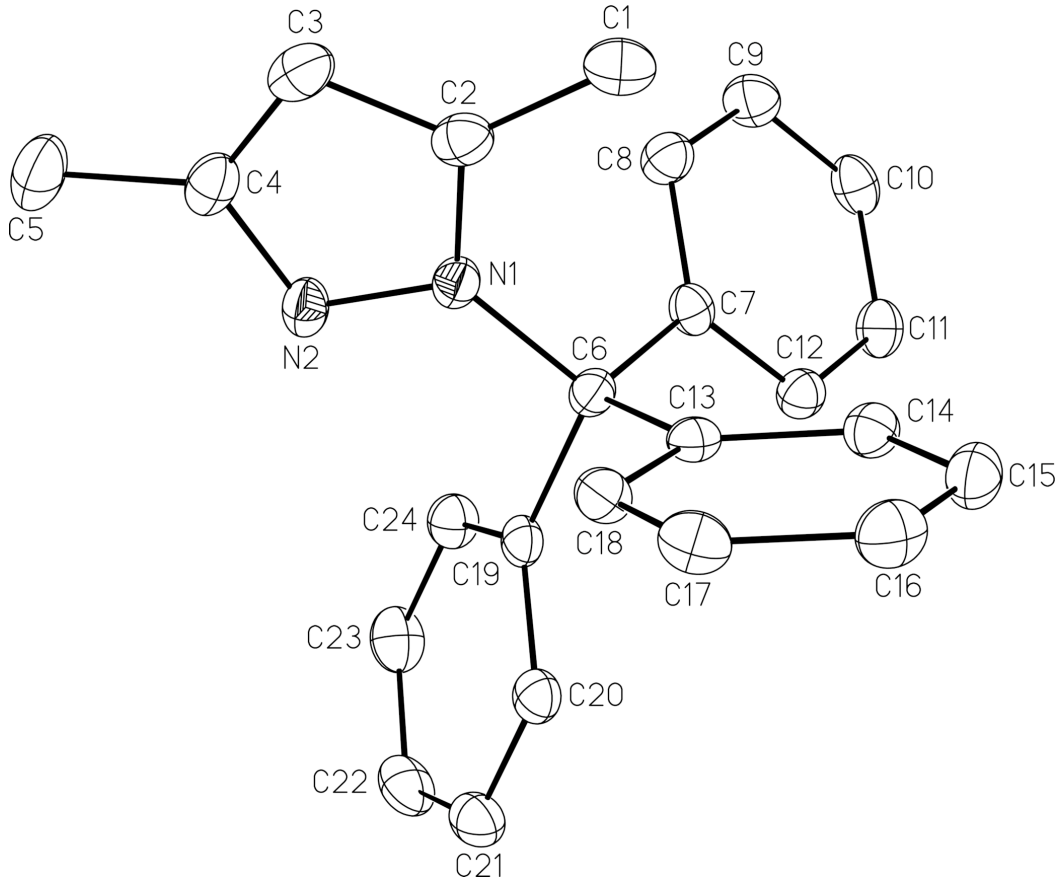
Geometric parameters (Å, °)

N1—C2	1.3673 (14)	C11—C12	1.3876 (16)
N1—N2	1.3690 (13)	C11—H11	0.9500
N1—C6	1.4950 (13)	C12—H12	0.9500
N2—C4	1.3299 (15)	C13—C14	1.3896 (15)
C1—C2	1.4914 (17)	C13—C18	1.4003 (15)
C1—H1A	0.9800	C14—C15	1.3955 (16)
C1—H1B	0.9800	C14—H14	0.9500
C1—H1C	0.9800	C15—C16	1.3839 (17)
C2—C3	1.3762 (16)	C15—H15	0.9500
C3—C4	1.4005 (18)	C16—C17	1.3912 (17)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.4997 (17)	C17—C18	1.3854 (16)
C5—H5A	0.9800	C17—H17	0.9500
C5—H5B	0.9800	C18—H18	0.9500
C5—H5C	0.9800	C19—C20	1.3882 (15)
C6—C7	1.5425 (15)	C19—C24	1.3991 (15)
C6—C13	1.5430 (14)	C20—C21	1.3948 (16)
C6—C19	1.5472 (15)	C20—H20	0.9500
C7—C8	1.3894 (16)	C21—C22	1.3792 (18)
C7—C12	1.3948 (16)	C21—H21	0.9500
C8—C9	1.3934 (17)	C22—C23	1.3916 (19)
C8—H8	0.9500	C22—H22	0.9500
C9—C10	1.3834 (17)	C23—C24	1.3842 (17)
C9—H9	0.9500	C23—H23	0.9500
C10—C11	1.3876 (17)	C24—H24	0.9500
C10—H10	0.9500		
C2—N1—N2	111.75 (9)	C10—C11—C12	120.48 (11)
C2—N1—C6	127.80 (9)	C10—C11—H11	119.8
N2—N1—C6	120.34 (9)	C12—C11—H11	119.8
C4—N2—N1	105.10 (9)	C11—C12—C7	120.98 (11)
C2—C1—H1A	109.5	C11—C12—H12	119.5
C2—C1—H1B	109.5	C7—C12—H12	119.5
H1A—C1—H1B	109.5	C14—C13—C18	118.24 (10)
C2—C1—H1C	109.5	C14—C13—C6	123.82 (10)
H1A—C1—H1C	109.5	C18—C13—C6	117.92 (9)
H1B—C1—H1C	109.5	C13—C14—C15	120.61 (10)
N1—C2—C3	105.83 (10)	C13—C14—H14	119.7
N1—C2—C1	126.20 (10)	C15—C14—H14	119.7
C3—C2—C1	127.97 (11)	C16—C15—C14	120.70 (11)
C2—C3—C4	106.31 (10)	C16—C15—H15	119.7
C2—C3—H3	126.8	C14—C15—H15	119.7
C4—C3—H3	126.8	C15—C16—C17	119.09 (10)
N2—C4—C3	111.00 (10)	C15—C16—H16	120.5

N2—C4—C5	120.36 (11)	C17—C16—H16	120.5
C3—C4—C5	128.64 (11)	C18—C17—C16	120.30 (11)
C4—C5—H5A	109.5	C18—C17—H17	119.9
C4—C5—H5B	109.5	C16—C17—H17	119.9
H5A—C5—H5B	109.5	C17—C18—C13	121.04 (10)
C4—C5—H5C	109.5	C17—C18—H18	119.5
H5A—C5—H5C	109.5	C13—C18—H18	119.5
H5B—C5—H5C	109.5	C20—C19—C24	118.04 (10)
N1—C6—C7	110.07 (8)	C20—C19—C6	122.66 (10)
N1—C6—C13	106.17 (8)	C24—C19—C6	119.22 (10)
C7—C6—C13	113.01 (9)	C19—C20—C21	120.94 (11)
N1—C6—C19	109.44 (8)	C19—C20—H20	119.5
C7—C6—C19	107.23 (8)	C21—C20—H20	119.5
C13—C6—C19	110.91 (8)	C22—C21—C20	120.39 (11)
C8—C7—C12	118.30 (10)	C22—C21—H21	119.8
C8—C7—C6	122.74 (10)	C20—C21—H21	119.8
C12—C7—C6	118.89 (9)	C21—C22—C23	119.30 (11)
C7—C8—C9	120.48 (11)	C21—C22—H22	120.4
C7—C8—H8	119.8	C23—C22—H22	120.4
C9—C8—H8	119.8	C24—C23—C22	120.23 (11)
C10—C9—C8	120.93 (11)	C24—C23—H23	119.9
C10—C9—H9	119.5	C22—C23—H23	119.9
C8—C9—H9	119.5	C23—C24—C19	121.04 (11)
C9—C10—C11	118.80 (11)	C23—C24—H24	119.5
C9—C10—H10	120.6	C19—C24—H24	119.5
C11—C10—H10	120.6		
C2—N1—N2—C4	−0.38 (12)	C8—C7—C12—C11	1.63 (16)
C6—N1—N2—C4	−177.00 (9)	C6—C7—C12—C11	178.94 (10)
N2—N1—C2—C3	0.20 (12)	N1—C6—C13—C14	−131.89 (10)
C6—N1—C2—C3	176.51 (10)	C7—C6—C13—C14	−11.14 (14)
N2—N1—C2—C1	179.95 (11)	C19—C6—C13—C14	109.30 (11)
C6—N1—C2—C1	−3.74 (18)	N1—C6—C13—C18	46.68 (12)
N1—C2—C3—C4	0.05 (12)	C7—C6—C13—C18	167.43 (9)
C1—C2—C3—C4	−179.69 (11)	C19—C6—C13—C18	−72.12 (12)
N1—N2—C4—C3	0.41 (12)	C18—C13—C14—C15	0.08 (16)
N1—N2—C4—C5	−179.94 (10)	C6—C13—C14—C15	178.65 (10)
C2—C3—C4—N2	−0.30 (13)	C13—C14—C15—C16	−0.94 (17)
C2—C3—C4—C5	−179.92 (12)	C14—C15—C16—C17	0.46 (17)
C2—N1—C6—C7	−73.89 (13)	C15—C16—C17—C18	0.88 (17)
N2—N1—C6—C7	102.14 (10)	C16—C17—C18—C13	−1.77 (17)
C2—N1—C6—C13	48.74 (13)	C14—C13—C18—C17	1.27 (16)
N2—N1—C6—C13	−135.22 (9)	C6—C13—C18—C17	−177.39 (10)
C2—N1—C6—C19	168.51 (10)	N1—C6—C19—C20	−113.81 (11)
N2—N1—C6—C19	−15.46 (13)	C7—C6—C19—C20	126.83 (10)
N1—C6—C7—C8	5.20 (14)	C13—C6—C19—C20	3.00 (14)
C13—C6—C7—C8	−113.30 (11)	N1—C6—C19—C24	69.65 (12)
C19—C6—C7—C8	124.17 (11)	C7—C6—C19—C24	−49.72 (12)
N1—C6—C7—C12	−171.98 (9)	C13—C6—C19—C24	−173.54 (9)
C13—C6—C7—C12	69.51 (12)	C24—C19—C20—C21	−1.72 (16)

C19—C6—C7—C12	−53.02 (12)	C6—C19—C20—C21	−178.31 (10)
C12—C7—C8—C9	−1.45 (16)	C19—C20—C21—C22	−0.68 (17)
C6—C7—C8—C9	−178.65 (10)	C20—C21—C22—C23	2.07 (18)
C7—C8—C9—C10	0.38 (18)	C21—C22—C23—C24	−1.02 (18)
C8—C9—C10—C11	0.54 (17)	C22—C23—C24—C19	−1.43 (18)
C9—C10—C11—C12	−0.37 (17)	C20—C19—C24—C23	2.78 (16)
C10—C11—C12—C7	−0.73 (17)	C6—C19—C24—C23	179.48 (10)

Fig. 1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