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1,3,5-Tricyclopropyl-1,3,5-triazinane

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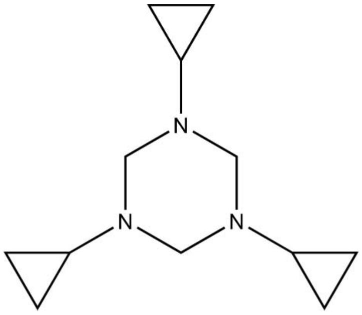
Key indicators: single-crystal X-ray study; T = 198 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.078; data-to-parameter ratio = 8.8.

The structure of the title compound, $C_{12}H_{21}N_3$, shows the most common conformation for free triazacyclohexanes, with one axial and two equatorial substituents at the nitrogen atoms. The N atoms show a distinctly pyramidal geometry, the N—C(cyclopropyl) bonds being inclined at 127.4 (2), 120.92 (19) and 121.32 (18)° to the CH_2—N—CH_2 plane. The biggest out-of-plane angle is found at the cyclopropane substituent in the axial position. The exocyclic C—N bonds at the equatorial sites are slightly longer than the one at the axial site. The C—C bond lengths in the cyclopropane rings range from 1.493 (3) to 1.503 (3) Å.

Related literature

For related literature, see: Adam *et al.* (1993); Adam *et al.* (1995); Ahrens, Herdtweck *et al.* (2006); Ahrens & Strassner (2006); Ahrens, Zeller *et al.* (2006); Anderson *et al.* (1995); Baker *et al.* (1999); Bouchemma *et al.* (1988); Bouchemma *et al.* (1989); Bouchemma *et al.* (1990); Bradley *et al.* (1992); Koehn *et al.* (2000); Koehn *et al.* (2005); Koehn *et al.* (1996); Laufer *et al.* (2002); Mloston *et al.* (2006); Muehlhofer, Strassner, Herdtweck & Herrmann (2002); Muehlhofer, Strassner & Herrmann (2002); Scheele *et al.* (2006); Sim (1987); Spek (2003); Strassner *et al.* (2004); Taige *et al.* (2007); Wilson *et al.* (2000); Wilson *et al.* (1999).



Experimental

Crystal data

$C_{12}H_{21}N_3$
M_r = 207.32
Orthorhombic, $Pna2_1$
a = 8.705 (1) Å
b = 16.231 (1) Å
c = 8.514 (2) Å
V = 1203.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 198 (2) K
0.55 × 0.15 × 0.07 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min}$ = 0.839, $T_{\max}$ = 0.995
7497 measured reflections
1191 independent reflections
1042 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.078
S = 1.04
1191 reflections
136 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.10 e Å^{-3}
$\Delta\rho_{\min}$ = −0.14 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SK3113).

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supplementary materials

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1,3,5-Tricyclopropyl-1,3,5-triazinane

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Comment

N,*N'*,*N''*-Trisubstituted 1,3,5-triazinanes are of interest as precursors for the preparation of different *N*-substituted imidazoles (Mloston *et al.*, 2006), which are building blocks for biologically active molecules *(Laufer et al., 2002)* or can be used as reactants for the preparation of *N*-heterocyclic carbenes, which are an interesting class of ligands in homogenous catalysis (Ahrens *et al.*, 2006a; Ahrens *et al.*, 2006 b, Ahrens *et al.*, 2006c, Muehlhofer *et al.*, 2002a, Muehlhofer *et al.*, 2002 b, Scheele *et al.*, 2006, Strassner *et al.*, 2004, Taige *et al.*, 2007). Furthermore 1,3,5-triazacyclohexanes are used as ligands in various metal complexes, *e.g.* in indium- (Bradley *et al.*, 1992), copper- and chromium- (Koehn *et al.*, 1996, Koehn *et al.*, 2000) or titanium complexes (Baker *et al.*, 1999, Koehn *et al.*, 2005, Wilson *et al.*, 1999, Wilson *et al.*, 2000).

The title compound (I) has been found as a byproduct during the formation of cyclopropylimidazole. The structure shows the most common conformation for free triazacyclohexanes with one axial and two equatorial cyclopropyl substituents at the nitrogen atoms as shown in Figure 1. The different conformational possibilities in dependence of various substituents at the nitrogen atoms of *N, N', N''*-substituted 1,3,5-triazanes have been studied in great detail by the groups of Anderson (Anderson *et al.*, 1995) and Sim (Sim, 1987, Bouchemma *et al.*, 1988, Bouchemma *et al.*, 1989, Bouchemma *et al.*, 1990, Adam *et al.* 1993, Adam *et al.* 1995).

In the solid state structure of (I) the C—N bond lengths are 1.442 (2) to 1.470 (2) Å, mean 1.455 Å, slightly shorter to those in the analogous 1,3,5-tricyclohexyl- (1.447 (2)–1.484 (2) Å, mean 1.463 Å) or the 1,3,5-tribenzyl-compound (1.445 (2)–1.480 (2) Å, mean 1.463 Å) (Bouchemma *et al.*, 1988). The N—CH_2—N angles range from 109.83 (18)° to 112.46 (15)°, which is nearly identical to the analogous 1,3,5-tricyclohexyl-1,3,5-triazinane (110.5 (2)°-112.9 (2)°). The CH_2—N—CH_2 angles in **1** (109.11 (15)° to 109.71 (14)°) are slightly bigger than in the solid state structure of the analogous cyclohexyl-compound (106.9 (2)°-109.1 (2)°).

Experimental

Paraformaldehyde (0.130 mol, 3.906 g) was suspended in 15 ml me thanol. Cyclopropylamine (0.124 mol, 7.074 g), dissolved in 15 ml me thanol, was added dropwise at 273 K. Ammonium carbonate (0.062 mol, 5.952 g) and a solution of 40% aqueous glyoxal (0.124 mol, 17.98 g) in 30 ml me thanol were added at 273 K. The reaction mixture was stirred at room temperature over night. Afterwards the solvent was removed *in vacuo* and the crude product was distilled at 388 K and 20 mbar. On cooling the title compound (I) crystallized in colorless plates from the yellow liquid and was separated by filtration.

Refinement

Preliminary examination and data collection were carried out on a Nonius *K*-CCD device with an Oxford Cryosystems cooling system at the window of a sealed X-ray tube with graphite-monochromated Mo—K_α radiation (λ = 0.71073 Å). After merging, all independent reflections were used to refine the structure. The structure was solved by a combination of direct methods and difference Fourier syntheses. All non-hydrogen atoms were refined with anisotropic displacement parameters. H atoms attached to carbon atoms were all positioned geometrically and treated as riding on their parent atoms, with C–H distances of 0.99 Å. The U_{iso}(H) values were set to 1.2 U_{eq}(C) for all C-bound H atoms. No useful absolute structure parameter could be refined, so Friedel-pair reflections were merged using the "MERG 3" instruction of *SHELXL-97* (Sheldrick, 1997) before final refinement. A calculation by *PLATON* (Spek, 2003) showed that there was no missed crystallographic symmetry.

Figures

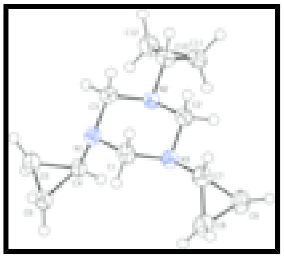

Fig. 1. A perspective view of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

1,3,5-tricyclopropyl-1,3,5-triazinane

Crystal data

$C_{12}H_{21}N_3$
$M_r = 207.32$
Orthorhombic, *Pna*2_1
Hall symbol: P 2c -2n
$a = 8.705$ (1) Å
$b = 16.231$ (1) Å
$c = 8.514$ (2) Å
$V = 1203.0$ (3) Å^3
$Z = 4$

$F_{000} = 456$
$D_x = 1.145$ Mg m^{-3}
Mo *K*α radiation
λ = 0.71073 Å
Cell parameters from 61 reflections
θ = 4.2–19.4°
μ = 0.07 mm^{-1}
$T = 198$ (2) K
Plate, colourless
0.55 × 0.15 × 0.07 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 9 pixels mm^{-1}
$T = 198(2)$ K
CCD scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.839$, $T_{max} = 0.995$
7497 measured reflections

1191 independent reflections
1042 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 25.4°$
$\theta_{min} = 3.6°$
$h = -10 \rightarrow 9$
$k = -19 \rightarrow 19$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.0772P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.078$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.10$ e Å^{-3}
1191 reflections	$\Delta\rho_{min} = -0.14$ e Å^{-3}
136 parameters	Extinction correction: none
1 restraint	Absolute structure: not possible
Primary atom site location: structure-invariant direct methods	Flack parameter: ?
Secondary atom site location: difference Fourier map	Rogers parameter: ?

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 > 2sigma(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.A multi-scan absorption correction was applied (absorption coefficient = 0.070 mm-1), and the maximum and minimum transmission factors were 0.9625 and 0.9951. Systematically absent reflections were not deleted and symmetry equivalent reflections were averaged to yield the set of unique data. No statistical outlier was deleted from the data set. The resulting 1191 data were used in the least squares refinement. The structure was solved using the SIR92 (Altomare *et al.*, 1993) software package. Subsequent least-squares refinement and difference Fourier calculations revealed the positions of the remaining non-hydrogen atoms. At this point, a calculation by PLATON (Spek, 2005) showed that there was no missed crystallographic symmetry. Nonhydrogen atoms were refined with independent anisotropic displacement parameters. H atoms attached to C atoms were all positioned geometrically and treated as riding on their parent atoms, with methyl C–H distances of 0.99 Å. The Uiso(H) values were set to 1.2 Ueq(C) for all C-bound H atoms. An isotropic extinction parameter (see the SHELX97 manual for the definition of the EXTI command) was not needed. The weighting parameters (see the SHELX97 manual for the definition of the WGHT command) were 0.0481 and 0.0772. Successful convergence was indicated by the maximum shift/error of 0.001 for the last cycle of least squares refinement. The largest peak in the final Fourier difference map (0.10 e Å-3) was located 1.37 Å from the H10 atom, deepest hole in the final Fourier difference map (-0.14 e Å-3) was located 1.08 Å from the C10 atom.

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

	x	y	z	U_{iso}*/U_{eq}
N1	0.82155 (17)	0.02211 (10)	0.50653 (19)	0.0287 (4)
N2	0.75402 (17)	−0.05661 (9)	0.73890 (19)	0.0281 (4)
N3	0.71919 (17)	0.08968 (8)	0.73811 (18)	0.0274 (4)
C1	0.8227 (2)	0.09588 (12)	0.6022 (2)	0.0322 (5)

C2	0.7634 (2)	0.01857 (12)	0.8333 (3)	0.0316 (5)
C3	0.8573 (2)	−0.04895 (12)	0.6031 (2)	0.0316 (5)
C4	0.6821 (2)	0.01260 (11)	0.4169 (2)	0.0286 (4)
C5	0.6958 (2)	−0.03324 (12)	0.2646 (3)	0.0361 (5)
C6	0.6747 (2)	0.05862 (12)	0.2644 (2)	0.0358 (5)
C7	0.7263 (2)	0.16415 (12)	0.8308 (2)	0.0340 (5)
C8	0.6263 (3)	0.23424 (12)	0.7814 (3)	0.0437 (5)
C9	0.5894 (3)	0.18672 (12)	0.9278 (2)	0.0401 (5)
C10	0.7969 (2)	−0.12719 (13)	0.8325 (2)	0.0369 (5)
C11	0.6753 (3)	−0.16634 (12)	0.9316 (3)	0.0426 (6)
C12	0.7319 (3)	−0.20850 (12)	0.7855 (3)	0.0484 (6)
H1A	0.6943	0.0140	0.9252	0.038*
H1B	0.8697	0.0259	0.8723	0.038*
H5A	0.8290	0.1789	0.8752	0.041*
H6A	0.9037	−0.1275	0.8759	0.044*
H7A	0.7915	0.1435	0.5369	0.039*
H7B	0.9286	0.1061	0.6399	0.039*
H8A	0.7641	0.0931	0.2351	0.043*
H8B	0.5738	0.0806	0.2310	0.043*
H9A	0.9645	−0.0444	0.6408	0.038*
H9B	0.8496	−0.0994	0.5382	0.038*
H10A	0.5841	0.0062	0.4769	0.034*
H11A	0.6078	0.2140	1.0301	0.048*
H11B	0.4996	0.1493	0.9253	0.048*
H12A	0.5711	−0.1418	0.9293	0.051*
H12B	0.7064	−0.1897	1.0342	0.051*
H13A	0.6077	−0.0677	0.2314	0.043*
H13B	0.7980	−0.0552	0.2355	0.043*
H14A	0.5592	0.2260	0.6888	0.052*
H14B	0.6673	0.2908	0.7936	0.052*
H15A	0.7976	−0.2578	0.7984	0.058*
H15B	0.6624	−0.2100	0.6935	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0276 (8)	0.0309 (8)	0.0276 (9)	−0.0001 (7)	0.0019 (8)	0.0004 (7)
N2	0.0333 (8)	0.0270 (8)	0.0240 (8)	0.0036 (6)	−0.0011 (7)	0.0007 (8)
N3	0.0315 (8)	0.0250 (8)	0.0255 (8)	−0.0033 (6)	−0.0005 (7)	−0.0019 (7)
C1	0.0328 (10)	0.0338 (11)	0.0301 (11)	−0.0065 (8)	0.0027 (9)	0.0011 (9)
C2	0.0328 (10)	0.0346 (11)	0.0275 (10)	−0.0002 (8)	−0.0024 (9)	0.0007 (9)
C3	0.0290 (9)	0.0352 (11)	0.0306 (10)	0.0074 (8)	0.0011 (9)	−0.0005 (9)
C4	0.0287 (10)	0.0325 (10)	0.0247 (10)	−0.0002 (8)	0.0031 (8)	−0.0011 (8)
C5	0.0434 (11)	0.0348 (10)	0.0302 (11)	−0.0016 (8)	0.0035 (10)	−0.0012 (9)
C6	0.0429 (11)	0.0359 (11)	0.0287 (11)	0.0041 (8)	0.0016 (9)	0.0024 (9)
C7	0.0386 (11)	0.0294 (11)	0.0342 (12)	−0.0070 (8)	−0.0025 (10)	−0.0055 (9)
C8	0.0632 (14)	0.0278 (10)	0.0402 (11)	0.0000 (9)	0.0016 (11)	−0.0046 (9)
C9	0.0531 (13)	0.0340 (10)	0.0331 (10)	−0.0046 (9)	0.0042 (10)	−0.0074 (9)

C10	0.0416 (11)	0.0361 (11)	0.0330 (11)	0.0109 (9)	−0.0036 (10)	0.0048 (9)
C11	0.0639 (14)	0.0332 (11)	0.0309 (11)	0.0101 (10)	0.0022 (11)	0.0091 (9)
C12	0.0779 (16)	0.0304 (11)	0.0370 (11)	0.0086 (10)	0.0002 (12)	0.0013 (11)

Geometric parameters (Å, °)

N1—C1	1.448 (2)	C6—C5	1.502 (3)
N1—C3	1.450 (2)	C6—H8A	0.9900
N1—C4	1.442 (2)	C6—H8B	0.9900
N2—C2	1.464 (2)	C7—C8	1.493 (3)
N2—C3	1.470 (2)	C7—C9	1.496 (3)
N2—C10	1.445 (2)	C7—H5A	1.0000
N3—C1	1.470 (2)	C8—H14A	0.9900
N3—C2	1.462 (2)	C8—H14B	0.9900
N3—C7	1.445 (2)	C9—C8	1.501 (3)
C1—H7A	0.9900	C9—H11A	0.9900
C1—H7B	0.9900	C9—H11B	0.9900
C2—H1A	0.9900	C10—C12	1.491 (3)
C2—H1B	0.9900	C10—C11	1.496 (3)
C3—H9A	0.9900	C10—H6A	1.0000
C3—H9B	0.9900	C11—C12	1.503 (3)
C4—C5	1.500 (3)	C11—H12A	0.9900
C4—H10A	1.0000	C11—H12B	0.9900
C5—H13A	0.9900	C12—H15A	0.9900
C5—H13B	0.9900	C12—H15B	0.9900
C6—C4	1.499 (3)		

N1—C1—N3	112.45 (14)	H8A—C6—H8B	114.9
N1—C3—N2	112.47 (15)	N1—C3—H9A	109.1
N1—C4—C5	116.36 (16)	N2—C3—H9A	109.1
N1—C4—C6	116.18 (16)	N1—C3—H9B	109.1
N1—C1—H7A	109.1	N2—C3—H9B	109.1
N1—C1—H7B	109.1	H9A—C3—H9B	107.8
N2—C2—H1A	109.7	N1—C4—H10A	117.3
N2—C2—H1B	109.7	C6—C4—H10A	117.3
N2—C10—C12	117.10 (18)	C5—C4—H10A	117.3
N2—C10—C11	117.71 (17)	C7—C9—C8	59.76 (14)
N2—C10—H6A	116.6	C7—C9—H11A	117.8
N3—C2—N2	109.81 (16)	C8—C9—H11A	117.8
N3—C7—C8	117.28 (17)	C7—C9—H11B	117.8
N3—C7—C9	118.19 (16)	C8—C9—H11B	117.8
N3—C2—H1A	109.7	H11A—C9—H11B	114.9
N3—C2—H1B	109.7	C10—C11—C12	59.63 (14)
N3—C7—H5A	116.4	C10—C11—H12A	117.8
N3—C1—H7A	109.1	C12—C11—H12A	117.8
N3—C1—H7B	109.1	C10—C11—H12B	117.8
C1—N1—C3	109.71 (15)	C12—C11—H12B	117.8
C2—N2—C3	109.10 (15)	H12A—C11—H12B	114.9
C2—N3—C1	109.20 (15)	C4—C5—C6	59.93 (13)
C4—N1—C1	113.08 (14)	C4—C5—H13A	117.8

C4—N1—C3	113.30 (14)	C6—C5—H13A	117.8
C4—C6—H8B	117.8	C4—C5—H13B	117.8
C4—C6—C5	59.95 (12)	C6—C5—H13B	117.8
C4—C6—H8A	117.8	H13A—C5—H13B	114.9
C5—C6—H8B	117.8	C7—C8—C9	59.94 (14)
C5—C6—H8A	117.8	C7—C8—H14A	117.8
C6—C4—C5	60.12 (13)	C9—C8—H14A	117.8
C7—N3—C2	110.26 (15)	C7—C8—H14B	117.8
C7—N3—C1	110.27 (14)	C9—C8—H14B	117.8
C8—C7—C9	60.30 (14)	H14A—C8—H14B	114.9
C8—C7—H5A	116.4	C10—C12—C11	59.95 (14)
C9—C7—H5A	116.4	C10—C12—H15A	117.8
C10—N2—C2	110.09 (16)	C11—C12—H15A	117.8
C10—N2—C3	110.07 (14)	C10—C12—H15B	117.8
C11—C10—H6A	116.6	C11—C12—H15B	117.8
C12—C10—C11	60.42 (14)	H1A—C2—H1B	108.2
C12—C10—H6A	116.6	H15A—C12—H15B	114.9
H7A—C1—H7B	107.8		

C7—N3—C2—N2	179.30 (15)	C3—N1—C1—N3	−55.09 (19)
C1—N3—C2—N2	−59.40 (18)	C7—N3—C1—N1	179.13 (15)
C10—N2—C2—N3	−179.73 (15)	C4—N1—C3—N2	−72.3 (2)
C3—N2—C2—N3	59.38 (18)	C1—N1—C3—N2	55.15 (19)
C2—N3—C7—C8	−154.53 (17)	C10—N2—C3—N1	−178.74 (16)
C1—N3—C7—C8	84.8 (2)	C2—N2—C3—N1	−57.84 (19)
C2—N3—C7—C9	−85.4 (2)	C3—N1—C4—C6	−151.14 (16)
C1—N3—C7—C9	153.95 (17)	C1—N1—C4—C5	151.15 (16)
C2—N2—C10—C12	153.83 (18)	C3—N1—C4—C5	−83.2 (2)
C3—N2—C10—C12	−85.9 (2)	C5—C6—C4—N1	106.75 (18)
C1—N1—C4—C6	83.23 (19)	N3—C7—C9—C8	−107.0 (2)
C2—N2—C10—C11	84.8 (2)	N2—C10—C11—C12	107.1 (2)
C2—N3—C1—N1	57.84 (19)	N1—C4—C5—C6	−106.44 (18)
C3—N2—C10—C11	−154.92 (18)	N3—C7—C8—C9	108.53 (19)
C4—N1—C1—N3	72.45 (19)	N2—C10—C12—C11	−108.1 (2)

Fig. 1