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N-Methyl-*N*-propyltryptamine (MPT)

Andrew R. Chadeayne,[a]* James A. Golen[b] and David R. Manke[b]

[a]CaaMTech, LLC, 58 East Sunset Way, Suite 209, Issaquah, WA 98027, USA, and [b]Department of Chemistry & Biochemistry, University of Massachusetts Dartmouth, 285 Old Westport Road, North Dartmouth, MA 02747, USA. *Correspondence e-mail: andrew@caam.tech

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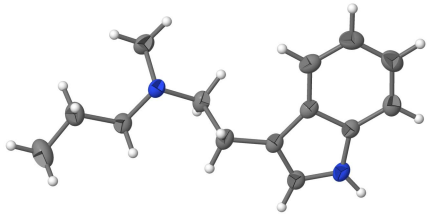
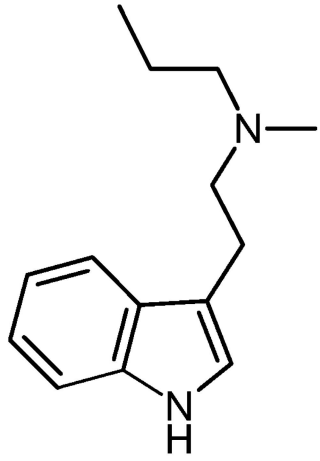
Structural data: full structural data are available from iucrdata.iucr.org

The title compound {systematic name: [2-(1*H*-indol-3-yl)ethyl](methyl)propylamine}, $C_{14}H_{20}N_2$, has a single molecule in the asymmetric unit. The molecules in the unit cell are held together in infinite one-dimensional chains along [010] through N—H···N hydrogen bonds between indole H atoms and trialkylamine N atoms.

3D view



Chemical scheme



Structure description

N-Methyl-*N*-propyltryptamine (MPT) is a structural analog of *N*,*N*-dimethyltryptamine (DMT), which is a well known 'psychedelic' molecule found in a variety of naturally occurring organisms, including plants, animals, and funghi, including mushrooms. In humans, DMT is the only known endogenous mammalian *N*,*N*-dimethylated trace amine (Fontanilla *et al.*, 2009). Naturally occurring tryptamines (*e.g.* DMT, psilocybin, 5-methoxy-*N*,*N*-dimethyltryptamine) and their synthetic derivatives (*e.g.* psilacetin, MPT) have garnered considerable attention of late due to new evidence demonstrating their efficacy in treating mood (*e.g.* anxiety and depression) and post traumatic stress disorders (PTSDs) (Aixalà *et al.*, 2018; Cameron *et al.*, 2019).

Psilocybin, isolated from the so-called 'magic' mushrooms, is perhaps the best known prodrug of the serotonin 2a agonist psilocin (Nichols, 2016). Recent studies indicate that psilocin (and its prodrugs like psilocybin and psilacetin) could provide effective treatment for mood disorders, end-of-life anxiety, addiction, and PTSD (Carhart-Harris *et al.*, 2016; Johnson & Griffiths, 2017). However, the long duration of action of psilocin and its prodrugs can result in practical challenges for both patients and clinicians (Passie *et al.*, 2002). Accordingly, the mental health industry would benefit from exploring alternative tryptamine treatment options that provide similar therapeutic benefits while having a shorter duration of action.

While the synthesis of DMT was first reported in 1931 (Manske, 1931), the first literature report of MPT appeared in 2005 (Brandt *et al.*, 2005) and it has not undergone significant study. In the solid-state structure of MPT, there is a single molecule in the asymmetric unit, with an indole group that demonstrates a mean deviation from planarity

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.920 (17)	1.990 (17)	2.9097 (15)	179.8 (16)

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$.

of 0.015 Å (Fig. 1). The metrical parameters are consistent with the previously reported structure of DMT (Falkenberg, 1972) and other dialkyltryptamines (Chadeayne *et al.*, 2019*a*,*b*; Petcher & Weber, 1974; Weber & Petcher, 1974). The tryptamine molecules are held together in an infinite one-dimensional chain along [010] through N—H···N hydrogen bonds connecting the indole N atom to the amine N atom (Table 1, Fig. 2). In the structure of DMT, there are similar hydrogen bonds, but they hold molecules together as dimers rather than in a chain. There are no π–π interactions observed in the structure.

Synthesis and crystallization

Single crystals of MPT suitable for X-ray analysis were obtained by the slow evaporation of a methylene chloride solution of a commercial sample of *N*-methyl-*N*-propyltryptamine (The Indole Shop).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

Financial statements and conflict of interest: This study was funded by CaaMTech, LLC. ARC reports an ownership interest in CaaMTech, LLC, which has filed patent applications covering compositions of psilocybin derivatives.

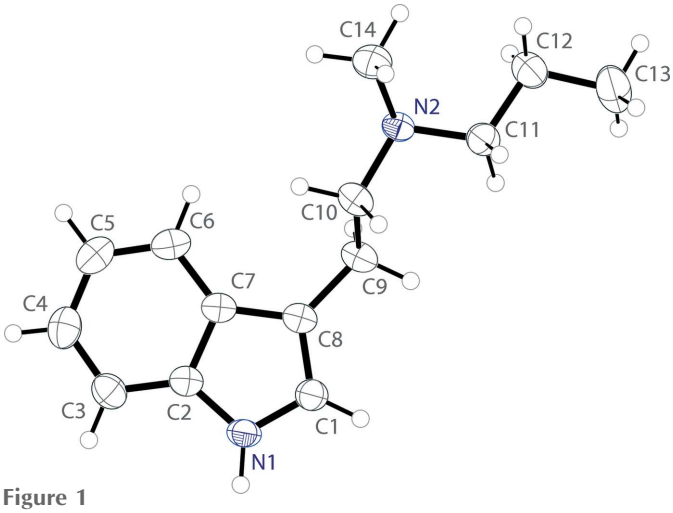


Figure 1
The molecular structure of the title compound, showing the atomic labelling. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{20}N_2$
M_r	216.32
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	200
a, *b*, *c* (Å)	13.5715 (11), 12.4352 (10), 15.1627 (12)
V (Å^3)	2558.9 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.28 × 0.20 × 0.13
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.713, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	47431, 2350, 1942
R_{int}	0.048
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.604
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.095, 1.05
No. of reflections	2350
No. of parameters	152
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.16

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *publCIF* (Westrip, 2010) and *OLEX2* (Dolomanov *et al.*, 2009).

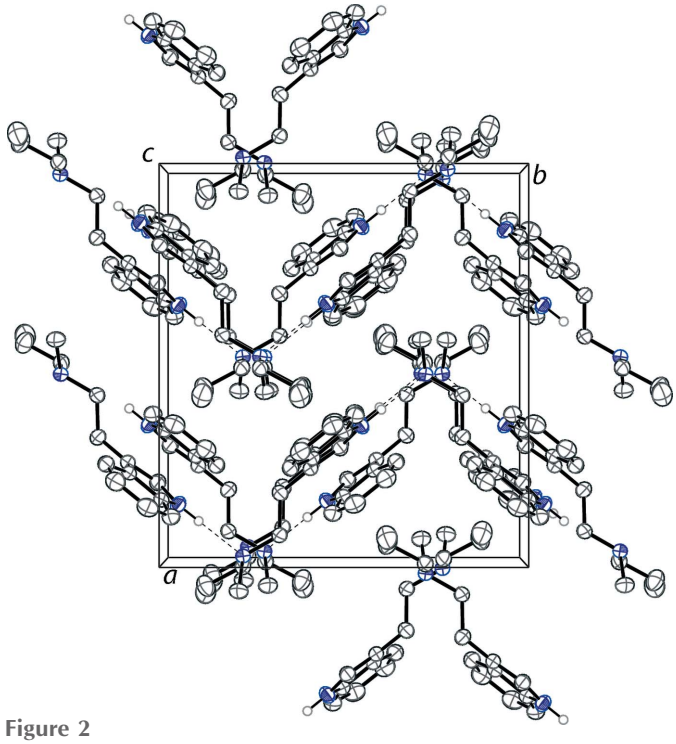


Figure 2
The crystal packing of the title compound, viewed along the *c* axis. The N—H···N hydrogen bonds are shown as dashed lines. Displacement ellipsoids are drawn at the 50% probability level. H atoms not involved in hydrogen bonding have been omitted for clarity.

Funding information

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full crystallographic data

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[2-(1*H*-Indol-3-yl)ethyl](methyl)propylamine

Crystal data

$C_{14}H_{20}N_2$
M_r = 216.32
Orthorhombic, *Pbca*
a = 13.5715 (11) Å
b = 12.4352 (10) Å
c = 15.1627 (12) Å
V = 2558.9 (4) Å^3
Z = 8
F(000) = 944
D_x = 1.123 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 9106 reflections
θ = 3.0–25.3°
μ = 0.07 mm^{-1}
T = 200 K
Block, colourless
0.28 × 0.20 × 0.13 mm

Data collection

Bruker D8 Venture CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.713, T_{max} = 0.745
47431 measured reflections
2350 independent reflections
1942 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.4°, θ_{min} = 3.0°
h = −16→16
k = −14→15
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
S = 1.05
2350 reflections
152 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.843P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0279 (16)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.15123 (8)	0.54678 (9)	0.71757 (7)	0.0342 (3)
N2	0.47825 (7)	0.22356 (7)	0.76631 (7)	0.0281 (3)
C1	0.20625 (9)	0.48945 (10)	0.77718 (8)	0.0329 (3)
H1A	0.2086	0.5040	0.8387	0.040*
C2	0.16536 (9)	0.50319 (10)	0.63560 (8)	0.0299 (3)
C3	0.12410 (10)	0.53092 (11)	0.55460 (9)	0.0380 (3)
H3	0.0802	0.5901	0.5494	0.046*
C4	0.14904 (10)	0.46983 (12)	0.48231 (9)	0.0438 (4)
H4	0.1221	0.4873	0.4263	0.053*
C7	0.23153 (8)	0.41566 (9)	0.64465 (8)	0.0291 (3)
C5	0.21333 (10)	0.38242 (12)	0.48980 (9)	0.0427 (4)
H5	0.2288	0.3413	0.4389	0.051*
C6	0.25456 (10)	0.35491 (11)	0.56941 (9)	0.0368 (3)
H6	0.2982	0.2954	0.5735	0.044*
C8	0.25697 (9)	0.40901 (9)	0.73654 (8)	0.0299 (3)
C9	0.32024 (9)	0.32514 (10)	0.77938 (9)	0.0347 (3)
H9A	0.2902	0.2536	0.7696	0.042*
H9B	0.3217	0.3382	0.8438	0.042*
C10	0.42572 (9)	0.32375 (10)	0.74460 (9)	0.0334 (3)
H10A	0.4245	0.3328	0.6797	0.040*
H10B	0.4622	0.3854	0.7699	0.040*
C11	0.50645 (10)	0.22182 (10)	0.85999 (8)	0.0341 (3)
H11A	0.4465	0.2323	0.8962	0.041*
H11B	0.5511	0.2832	0.8716	0.041*
C12	0.55691 (12)	0.11938 (12)	0.88919 (10)	0.0473 (4)
H12A	0.6211	0.1130	0.8585	0.057*
H12B	0.5159	0.0570	0.8719	0.057*
C13	0.57384 (14)	0.11646 (13)	0.98776 (10)	0.0574 (4)
H13A	0.6089	0.0503	1.0034	0.086*
H13B	0.5103	0.1184	1.0183	0.086*
H13C	0.6133	0.1789	1.0054	0.086*
C14	0.56449 (10)	0.21237 (11)	0.70873 (9)	0.0402 (3)
H14A	0.5432	0.2125	0.6470	0.060*
H14B	0.5982	0.1446	0.7219	0.060*
H14C	0.6097	0.2726	0.7189	0.060*
H1	0.1103 (12)	0.6027 (13)	0.7328 (10)	0.055 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0332 (6)	0.0297 (6)	0.0396 (6)	0.0077 (5)	−0.0033 (5)	−0.0054 (5)
N2	0.0232 (5)	0.0262 (5)	0.0350 (6)	−0.0004 (4)	−0.0003 (4)	−0.0002 (4)
C1	0.0321 (6)	0.0317 (7)	0.0350 (7)	0.0017 (5)	−0.0026 (5)	−0.0024 (5)
C2	0.0248 (6)	0.0282 (6)	0.0365 (7)	−0.0018 (5)	0.0000 (5)	−0.0019 (5)
C3	0.0322 (7)	0.0386 (7)	0.0434 (8)	0.0002 (6)	−0.0045 (6)	0.0023 (6)

C4	0.0412 (8)	0.0546 (9)	0.0356 (8)	−0.0068 (7)	−0.0034 (6)	0.0001 (6)
C7	0.0231 (6)	0.0255 (6)	0.0386 (7)	−0.0031 (5)	0.0019 (5)	−0.0019 (5)
C5	0.0422 (8)	0.0479 (8)	0.0380 (8)	−0.0059 (6)	0.0052 (6)	−0.0103 (6)
C6	0.0320 (7)	0.0335 (7)	0.0448 (8)	−0.0010 (5)	0.0055 (6)	−0.0074 (6)
C8	0.0252 (6)	0.0263 (6)	0.0383 (7)	−0.0011 (5)	0.0005 (5)	0.0000 (5)
C9	0.0298 (7)	0.0302 (7)	0.0442 (8)	0.0033 (5)	0.0023 (6)	0.0047 (5)
C10	0.0273 (6)	0.0286 (6)	0.0441 (7)	−0.0015 (5)	−0.0006 (5)	0.0065 (5)
C11	0.0339 (7)	0.0307 (7)	0.0377 (7)	−0.0007 (5)	−0.0048 (5)	−0.0025 (5)
C12	0.0545 (9)	0.0413 (8)	0.0462 (8)	0.0095 (7)	−0.0089 (7)	0.0019 (6)
C13	0.0701 (11)	0.0508 (9)	0.0514 (9)	−0.0043 (8)	−0.0200 (8)	0.0090 (7)
C14	0.0288 (7)	0.0439 (8)	0.0478 (8)	0.0014 (6)	0.0060 (6)	0.0007 (6)

Geometric parameters (Å, º)

N1—C1	1.3722 (16)	C8—C9	1.4991 (17)
N1—C2	1.3695 (16)	C9—H9A	0.9900
N1—H1	0.920 (17)	C9—H9B	0.9900
N2—C10	1.4727 (15)	C9—C10	1.5257 (17)
N2—C11	1.4712 (15)	C10—H10A	0.9900
N2—C14	1.4668 (16)	C10—H10B	0.9900
C1—H1A	0.9500	C11—H11A	0.9900
C1—C8	1.3618 (17)	C11—H11B	0.9900
C2—C3	1.3932 (18)	C11—C12	1.5126 (18)
C2—C7	1.4177 (17)	C12—H12A	0.9900
C3—H3	0.9500	C12—H12B	0.9900
C3—C4	1.3759 (19)	C12—C13	1.513 (2)
C4—H4	0.9500	C13—H13A	0.9800
C4—C5	1.398 (2)	C13—H13B	0.9800
C7—C6	1.4035 (17)	C13—H13C	0.9800
C7—C8	1.4377 (18)	C14—H14A	0.9800
C5—H5	0.9500	C14—H14B	0.9800
C5—C6	1.374 (2)	C14—H14C	0.9800
C6—H6	0.9500		
C1—N1—H1	123.8 (10)	H9A—C9—H9B	107.7
C2—N1—C1	108.42 (10)	C10—C9—H9A	108.9
C2—N1—H1	127.7 (10)	C10—C9—H9B	108.9
C11—N2—C10	110.74 (10)	N2—C10—C9	112.74 (10)
C14—N2—C10	109.48 (10)	N2—C10—H10A	109.0
C14—N2—C11	111.45 (10)	N2—C10—H10B	109.0
N1—C1—H1A	124.5	C9—C10—H10A	109.0
C8—C1—N1	111.01 (11)	C9—C10—H10B	109.0
C8—C1—H1A	124.5	H10A—C10—H10B	107.8
N1—C2—C3	130.23 (12)	N2—C11—H11A	108.7
N1—C2—C7	107.74 (11)	N2—C11—H11B	108.7
C3—C2—C7	122.01 (12)	N2—C11—C12	114.38 (10)
C2—C3—H3	121.1	H11A—C11—H11B	107.6
C4—C3—C2	117.83 (13)	C12—C11—H11A	108.7

C4—C3—H3	121.1	C12—C11—H11B	108.7
C3—C4—H4	119.4	C11—C12—H12A	109.2
C3—C4—C5	121.19 (13)	C11—C12—H12B	109.2
C5—C4—H4	119.4	C11—C12—C13	112.22 (12)
C2—C7—C8	106.87 (10)	H12A—C12—H12B	107.9
C6—C7—C2	118.39 (11)	C13—C12—H12A	109.2
C6—C7—C8	134.69 (12)	C13—C12—H12B	109.2
C4—C5—H5	119.4	C12—C13—H13A	109.5
C6—C5—C4	121.27 (13)	C12—C13—H13B	109.5
C6—C5—H5	119.4	C12—C13—H13C	109.5
C7—C6—H6	120.3	H13A—C13—H13B	109.5
C5—C6—C7	119.31 (12)	H13A—C13—H13C	109.5
C5—C6—H6	120.3	H13B—C13—H13C	109.5
C1—C8—C7	105.96 (10)	N2—C14—H14A	109.5
C1—C8—C9	127.19 (12)	N2—C14—H14B	109.5
C7—C8—C9	126.70 (11)	N2—C14—H14C	109.5
C8—C9—H9A	108.9	H14A—C14—H14B	109.5
C8—C9—H9B	108.9	H14A—C14—H14C	109.5
C8—C9—C10	113.30 (10)	H14B—C14—H14C	109.5
N1—C1—C8—C7	−0.41 (14)	C3—C2—C7—C6	−0.82 (18)
N1—C1—C8—C9	−176.10 (11)	C3—C2—C7—C8	−178.57 (11)
N1—C2—C3—C4	−177.51 (13)	C3—C4—C5—C6	−0.5 (2)
N1—C2—C7—C6	177.50 (11)	C4—C5—C6—C7	0.1 (2)
N1—C2—C7—C8	−0.25 (13)	C7—C2—C3—C4	0.40 (19)
N2—C11—C12—C13	−173.49 (12)	C7—C8—C9—C10	62.03 (17)
C1—N1—C2—C3	178.13 (13)	C6—C7—C8—C1	−176.81 (13)
C1—N1—C2—C7	0.00 (14)	C6—C7—C8—C9	−1.1 (2)
C1—C8—C9—C10	−123.14 (14)	C8—C7—C6—C5	177.52 (13)
C2—N1—C1—C8	0.27 (14)	C8—C9—C10—N2	−162.95 (10)
C2—C3—C4—C5	0.3 (2)	C10—N2—C11—C12	177.40 (11)
C2—C7—C6—C5	0.56 (18)	C11—N2—C10—C9	−74.78 (13)
C2—C7—C8—C1	0.40 (13)	C14—N2—C10—C9	161.94 (11)
C2—C7—C8—C9	176.12 (11)	C14—N2—C11—C12	−60.47 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.920 (17)	1.990 (17)	2.9097 (15)	179.8 (16)

Symmetry code: (i) −*x*+1/2, *y*+1/2, *z*.