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# 6-Methyl-*N*-(2-methylphenyl)-3-phenyl-1,6-dihydro-1,2,4,5-tetrazine-1-carboxamide. Corrigendum

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Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; H-atom completeness 95%; $R$ factor = 0.064; $wR$ factor = 0.170; data-to-parameter ratio = 15.3.

The formula of the title compound in the paper by Xu & Hu [*Acta Cryst.* (2008), E**64**, o1432] is corrected.

In the paper by Xu & Hu [*Acta Cryst.* (2008), E**64**, o1432], the chemical formula is corrected and the structure has been rerefined to include a missing H atom. The *Crystal data*, *Data collection* and *Refinement* sections are updated together with the hydrogen-bond data.

## Experimental

### *Crystal data*

$C_{17}H_{17}N_5O$
$M_r$ = 307.36
Monoclinic, $P2_1/c$
$a$ = 13.941 (6) Å
$b$ = 5.675 (2) Å
$c$ = 20.614 (8) Å
$\beta$ = 102.055 (6)°
$V$ = 1594.8 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 (2) K
0.12 × 0.10 × 0.06 mm

### *Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.990, $T_{max}$ = 0.995
7095 measured reflections
3280 independent reflections
1899 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.087

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.170
$S$ = 0.91
3280 reflections
215 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C6—H6···O$^{i}$ | 0.93 | 2.56 | 3.385 (3) | 148 |

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

## References

Xu, F. & Hu, W. (2008). *Acta Cryst.* E**64**, o1432.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

# supporting information

*Acta Cryst.* (2010). E**66**, e15 [https://doi.org/10.1107/S160053680903013X]

## 6-Methyl-*N*-(2-methylphenyl)-3-phenyl-1,6-dihydro-1,2,4,5-tetrazine-1-carboxamide. Corrigendum

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*Crystal data*

$C_{17}H_{17}N_5O$
$M_r = 307.36$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.941$ (6) Å
$b = 5.675$ (2) Å
$c = 20.614$ (8) Å
$\beta = 102.055$ (6)°
$V = 1594.8$ (11) Å$^3$
$Z = 4$
$F(000) = 644$
$D_x = 1.276$ Mg m$^{-3}$
Melting point = 378–380 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 742 reflections
$\theta = 3.2$–24.8°
$\mu = 0.08$ mm$^{-1}$
$T = 293$ K
Prism, red
0.12 × 0.10 × 0.06 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.990$, $T_{max} = 0.995$
7095 measured reflections
3280 independent reflections
1899 reflections with $I > 2\sigma(I)$
$R_{int} = 0.087$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.5°$
$h = -17\rightarrow8$
$k = -6\rightarrow7$
$l = -25\rightarrow25$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.170$
$S = 0.91$
3280 reflections
215 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0932P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.54$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ e Å$^{-3}$
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.021 (4)

*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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O | 0.79549 (13) | 0.2358 (3) | 0.73526 (8) | 0.0685 (5) |
| N1 | 0.82379 (14) | 0.4541 (3) | 0.64939 (9) | 0.0552 (5) |
| N2 | 0.79315 (13) | 0.5181 (3) | 0.58485 (9) | 0.0522 (5) |
| N3 | 0.88534 (17) | 0.8632 (4) | 0.61618 (12) | 0.0685 (6) |
| N4 | 0.91853 (17) | 0.7948 (4) | 0.67409 (12) | 0.0724 (6) |
| N5 | 0.68918 (15) | 0.2115 (4) | 0.63448 (10) | 0.0598 (6) |
| H5N | 0.6759 (17) | 0.282 (4) | 0.5967 (12) | 0.054 (6)* |
| C1 | 0.91906 (18) | 0.5354 (4) | 0.68427 (11) | 0.0587 (6) |
| C2 | 0.83633 (17) | 0.7032 (4) | 0.56768 (11) | 0.0526 (6) |
| C3 | 0.82173 (17) | 0.7755 (4) | 0.49788 (12) | 0.0542 (6) |
| C4 | 0.77371 (19) | 0.6256 (5) | 0.44798 (12) | 0.0644 (7) |
| H4 | 0.7490 | 0.4824 | 0.4592 | 0.077* |
| C5 | 0.7624 (2) | 0.6873 (6) | 0.38197 (14) | 0.0813 (9) |
| H5 | 0.7307 | 0.5853 | 0.3491 | 0.098* |
| C6 | 0.7975 (2) | 0.8971 (6) | 0.36496 (16) | 0.0825 (9) |
| H6 | 0.7889 | 0.9392 | 0.3205 | 0.099* |
| C7 | 0.8452 (3) | 1.0452 (6) | 0.41287 (18) | 0.0876 (10) |
| H7 | 0.8701 | 1.1870 | 0.4009 | 0.105* |
| C8 | 0.8571 (2) | 0.9862 (5) | 0.47985 (15) | 0.0788 (8) |
| H8 | 0.8889 | 1.0897 | 0.5123 | 0.095* |
| C9 | 0.76906 (18) | 0.2904 (4) | 0.67787 (11) | 0.0535 (6) |
| C10 | 0.61865 (18) | 0.0506 (4) | 0.64801 (11) | 0.0559 (6) |
| C11 | 0.6437 (2) | −0.1223 (5) | 0.69669 (13) | 0.0724 (8) |
| H11 | 0.7077 | −0.1329 | 0.7210 | 0.087* |
| C12 | 0.5740 (3) | −0.2762 (6) | 0.70856 (15) | 0.0883 (10) |
| H12 | 0.5905 | −0.3910 | 0.7412 | 0.106* |
| C13 | 0.4807 (3) | −0.2619 (6) | 0.67292 (18) | 0.0928 (11) |
| H13 | 0.4330 | −0.3646 | 0.6817 | 0.111* |
| C14 | 0.4564 (2) | −0.0944 (6) | 0.62345 (16) | 0.0817 (9) |
| H14 | 0.3926 | −0.0891 | 0.5987 | 0.098* |
| C15 | 0.52429 (19) | 0.0652 (4) | 0.60974 (12) | 0.0601 (7) |
| C16 | 1.00241 (18) | 0.4238 (5) | 0.65920 (13) | 0.0658 (7) |
| H16A | 1.0013 | 0.2564 | 0.6656 | 0.099* |
| H16B | 1.0636 | 0.4865 | 0.6832 | 0.099* |
| H16C | 0.9955 | 0.4575 | 0.6128 | 0.099* |

| | | | | |
|---|---|---|---|---|
| C17 | 0.4969 (3) | 0.2482 (6) | 0.55605 (17) | 0.0790 (8) |
| H17A | 0.431 (3) | 0.232 (5) | 0.5290 (16) | 0.102 (10)* |
| H17B | 0.543 (2) | 0.223 (5) | 0.5212 (15) | 0.092 (9)* |
| H17C | 0.511 (3) | 0.408 (7) | 0.5726 (16) | 0.107 (11)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O | 0.0755 (12) | 0.0808 (13) | 0.0475 (10) | −0.0050 (9) | 0.0090 (8) | 0.0014 (7) |
| N1 | 0.0491 (11) | 0.0653 (12) | 0.0486 (10) | −0.0056 (10) | 0.0039 (8) | 0.0001 (8) |
| N2 | 0.0469 (11) | 0.0556 (11) | 0.0529 (11) | −0.0018 (9) | 0.0077 (8) | 0.0026 (8) |
| N3 | 0.0682 (14) | 0.0511 (12) | 0.0823 (15) | −0.0009 (10) | 0.0067 (12) | −0.0101 (10) |
| N4 | 0.0740 (15) | 0.0636 (14) | 0.0742 (15) | −0.0012 (11) | 0.0030 (12) | −0.0181 (11) |
| N5 | 0.0537 (12) | 0.0737 (14) | 0.0501 (12) | −0.0109 (10) | 0.0064 (10) | 0.0102 (9) |
| C1 | 0.0521 (15) | 0.0578 (14) | 0.0616 (14) | −0.0068 (12) | 0.0015 (11) | −0.0095 (10) |
| C2 | 0.0488 (13) | 0.0424 (12) | 0.0658 (14) | 0.0002 (11) | 0.0098 (11) | −0.0017 (9) |
| C3 | 0.0427 (13) | 0.0485 (13) | 0.0722 (15) | 0.0022 (10) | 0.0137 (11) | 0.0085 (10) |
| C4 | 0.0610 (16) | 0.0681 (16) | 0.0637 (15) | −0.0068 (13) | 0.0123 (12) | 0.0116 (11) |
| C5 | 0.0763 (19) | 0.101 (2) | 0.0649 (16) | −0.0060 (17) | 0.0117 (14) | 0.0133 (14) |
| C6 | 0.0736 (19) | 0.095 (2) | 0.0832 (19) | 0.0109 (18) | 0.0271 (16) | 0.0321 (17) |
| C7 | 0.094 (2) | 0.0653 (19) | 0.115 (3) | −0.0012 (17) | 0.047 (2) | 0.0308 (17) |
| C8 | 0.084 (2) | 0.0583 (17) | 0.098 (2) | −0.0070 (15) | 0.0271 (16) | 0.0097 (14) |
| C9 | 0.0520 (14) | 0.0604 (14) | 0.0484 (13) | 0.0014 (11) | 0.0111 (11) | −0.0033 (10) |
| C10 | 0.0597 (15) | 0.0570 (14) | 0.0548 (13) | −0.0092 (12) | 0.0210 (11) | −0.0027 (10) |
| C11 | 0.0846 (19) | 0.0703 (17) | 0.0646 (15) | −0.0100 (15) | 0.0209 (14) | 0.0082 (12) |
| C12 | 0.119 (3) | 0.080 (2) | 0.0732 (18) | −0.028 (2) | 0.035 (2) | 0.0027 (14) |
| C13 | 0.106 (3) | 0.089 (2) | 0.097 (2) | −0.042 (2) | 0.053 (2) | −0.0174 (18) |
| C14 | 0.0644 (18) | 0.090 (2) | 0.096 (2) | −0.0193 (16) | 0.0277 (16) | −0.0261 (17) |
| C15 | 0.0571 (16) | 0.0621 (15) | 0.0645 (14) | −0.0049 (12) | 0.0205 (12) | −0.0115 (11) |
| C16 | 0.0513 (15) | 0.0635 (16) | 0.0779 (16) | −0.0031 (12) | 0.0029 (12) | 0.0007 (11) |
| C17 | 0.064 (2) | 0.078 (2) | 0.087 (2) | 0.0031 (17) | −0.0032 (17) | −0.0037 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O—C9 | 1.204 (3) | C7—C8 | 1.397 (4) |
| N1—N2 | 1.359 (3) | C7—H7 | 0.9300 |
| N1—C9 | 1.406 (3) | C8—H8 | 0.9300 |
| N1—C1 | 1.447 (3) | C10—C15 | 1.388 (4) |
| N2—C2 | 1.296 (3) | C10—C11 | 1.395 (4) |
| N3—N4 | 1.249 (3) | C11—C12 | 1.366 (4) |
| N3—C2 | 1.416 (3) | C11—H11 | 0.9300 |
| N4—C1 | 1.487 (3) | C12—C13 | 1.356 (5) |
| N5—C9 | 1.351 (3) | C12—H12 | 0.9300 |
| N5—C10 | 1.412 (3) | C13—C14 | 1.383 (5) |
| N5—H5N | 0.86 (2) | C13—H13 | 0.9300 |
| C1—C16 | 1.506 (3) | C14—C15 | 1.381 (4) |
| C2—C3 | 1.469 (3) | C14—H14 | 0.9300 |
| C3—C8 | 1.374 (4) | C15—C17 | 1.508 (4) |

| | | | |
|---|---|---|---|
| C3—C4 | 1.394 (4) | C16—H16A | 0.9600 |
| C4—C5 | 1.382 (4) | C16—H16B | 0.9600 |
| C4—H4 | 0.9300 | C16—H16C | 0.9600 |
| C5—C6 | 1.361 (4) | C17—H17A | 0.98 (4) |
| C5—H5 | 0.9300 | C17—H17B | 1.07 (3) |
| C6—C7 | 1.360 (5) | C17—H17C | 0.97 (4) |
| C6—H6 | 0.9300 | | |

| | | | |
|---|---|---|---|
| N2—N1—C9 | 119.9 (2) | O—C9—N5 | 127.3 (2) |
| N2—N1—C1 | 118.0 (2) | O—C9—N1 | 119.9 (2) |
| C9—N1—C1 | 121.7 (2) | N5—C9—N1 | 112.8 (2) |
| C2—N2—N1 | 114.5 (2) | C15—C10—C11 | 121.1 (2) |
| N4—N3—C2 | 120.2 (2) | C15—C10—N5 | 117.7 (2) |
| N3—N4—C1 | 115.6 (2) | C11—C10—N5 | 121.1 (2) |
| C9—N5—C10 | 126.5 (2) | C12—C11—C10 | 119.9 (3) |
| C9—N5—H5N | 115.8 (16) | C12—C11—H11 | 120.1 |
| C10—N5—H5N | 117.0 (16) | C10—C11—H11 | 120.1 |
| N1—C1—N4 | 105.6 (2) | C13—C12—C11 | 120.2 (3) |
| N1—C1—C16 | 112.9 (2) | C13—C12—H12 | 119.9 |
| N4—C1—C16 | 110.4 (2) | C11—C12—H12 | 119.9 |
| N2—C2—N3 | 120.7 (2) | C12—C13—C14 | 120.0 (3) |
| N2—C2—C3 | 121.1 (2) | C12—C13—H13 | 120.0 |
| N3—C2—C3 | 117.4 (2) | C14—C13—H13 | 120.0 |
| C8—C3—C4 | 118.4 (2) | C15—C14—C13 | 122.0 (3) |
| C8—C3—C2 | 121.6 (2) | C15—C14—H14 | 119.0 |
| C4—C3—C2 | 120.0 (2) | C13—C14—H14 | 119.0 |
| C5—C4—C3 | 120.7 (2) | C14—C15—C10 | 116.9 (2) |
| C5—C4—H4 | 119.7 | C14—C15—C17 | 121.5 (3) |
| C3—C4—H4 | 119.7 | C10—C15—C17 | 121.5 (2) |
| C6—C5—C4 | 120.2 (3) | C1—C16—H16A | 109.5 |
| C6—C5—H5 | 119.9 | C1—C16—H16B | 109.5 |
| C4—C5—H5 | 119.9 | H16A—C16—H16B | 109.5 |
| C7—C6—C5 | 120.1 (3) | C1—C16—H16C | 109.5 |
| C7—C6—H6 | 120.0 | H16A—C16—H16C | 109.5 |
| C5—C6—H6 | 120.0 | H16B—C16—H16C | 109.5 |
| C6—C7—C8 | 120.6 (3) | C15—C17—H17A | 114.5 (19) |
| C6—C7—H7 | 119.7 | C15—C17—H17B | 107.6 (16) |
| C8—C7—H7 | 119.7 | H17A—C17—H17B | 104 (2) |
| C3—C8—C7 | 120.1 (3) | C15—C17—H17C | 112.6 (19) |
| C3—C8—H8 | 120.0 | H17A—C17—H17C | 113 (3) |
| C7—C8—H8 | 120.0 | H17B—C17—H17C | 105 (3) |

| | | | |
|---|---|---|---|
| C9—N1—N2—C2 | 166.3 (2) | C4—C3—C8—C7 | −0.5 (4) |
| C1—N1—N2—C2 | −21.5 (3) | C2—C3—C8—C7 | 177.5 (3) |
| C2—N3—N4—C1 | 10.6 (3) | C6—C7—C8—C3 | 1.0 (5) |
| N2—N1—C1—N4 | 52.3 (3) | C10—N5—C9—O | 1.3 (4) |
| C9—N1—C1—N4 | −135.5 (2) | C10—N5—C9—N1 | −178.6 (2) |
| N2—N1—C1—C16 | −68.4 (3) | N2—N1—C9—O | −179.1 (2) |

| | | | |
|---|---|---|---|
| C9—N1—C1—C16 | 103.7 (2) | C1—N1—C9—O | 8.9 (3) |
| N3—N4—C1—N1 | −45.4 (3) | N2—N1—C9—N5 | 0.8 (3) |
| N3—N4—C1—C16 | 77.0 (3) | C1—N1—C9—N5 | −171.2 (2) |
| N1—N2—C2—N3 | −19.4 (3) | C9—N5—C10—C15 | 152.7 (2) |
| N1—N2—C2—C3 | 171.32 (19) | C9—N5—C10—C11 | −29.4 (4) |
| N4—N3—C2—N2 | 25.8 (3) | C15—C10—C11—C12 | −2.0 (4) |
| N4—N3—C2—C3 | −164.6 (2) | N5—C10—C11—C12 | −179.8 (2) |
| N2—C2—C3—C8 | 171.8 (2) | C10—C11—C12—C13 | 0.3 (4) |
| N3—C2—C3—C8 | 2.2 (3) | C11—C12—C13—C14 | 1.4 (5) |
| N2—C2—C3—C4 | −10.2 (4) | C12—C13—C14—C15 | −1.6 (5) |
| N3—C2—C3—C4 | −179.8 (2) | C13—C14—C15—C10 | 0.0 (4) |
| C8—C3—C4—C5 | 0.3 (4) | C13—C14—C15—C17 | −179.5 (3) |
| C2—C3—C4—C5 | −177.7 (2) | C11—C10—C15—C14 | 1.8 (3) |
| C3—C4—C5—C6 | −0.5 (4) | N5—C10—C15—C14 | 179.7 (2) |
| C4—C5—C6—C7 | 1.0 (5) | C11—C10—C15—C17 | −178.7 (3) |
| C5—C6—C7—C8 | −1.2 (5) | N5—C10—C15—C17 | −0.8 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C6—H6···O$^{i}$ | 0.93 | 2.56 | 3.385 (3) | 148 |

Symmetry code: (i) $x$, $-y+3/2$, $z-1/2$.