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# *catena*-Poly[bis($\mu_4$-adipato-1:2:1′:2′$\kappa^4O^1$:$O^{1'}$:$O^4$:$O^{4'}$)bis(*N*,*N*-dimethylformamide)-1$\kappa O$,2$\kappa O$-dicopper(II)]

**Guo-Yun Wu[a] and Seik Weng Ng[b]***

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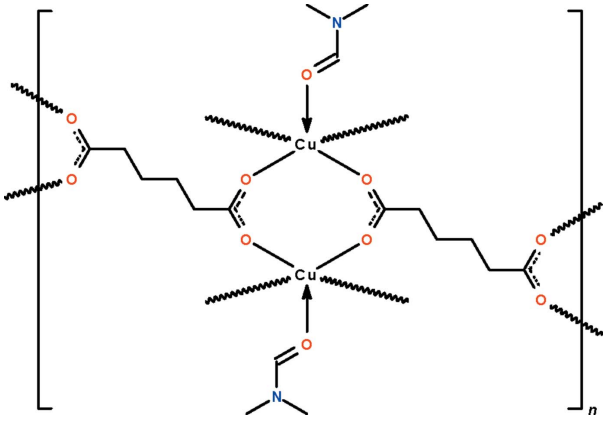
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.024; $wR$ factor = 0.072; data-to-parameter ratio = 16.5.

In the title polymeric complex, $[Cu_2(C_6H_8O_4)_2(C_3H_7NO)_2]_n$, the carboxylate groups of the approximately *U*-shaped adipate dianion each bridge a pair of inversion-related, DMF-coordinated copper(II) atoms, generating a ribbon motif that runs along the *b* axis. The geometry of the copper(II) atom is distorted square-pyramidal; the apical site is occupied by the O atom of the DMF molecule whereas the four basal sites are occupied by carboxylate O atoms.

## Related literature

For the crystal structure of diaquaadipatocopper(II), see: Bakalbassis *et al.* (2001); Zheng *et al.* (2001).




## Experimental

### Crystal data

$[Cu_2(C_6H_8O_4)_2(C_3H_7NO)_2]$
$M_r$ = 561.52
Monoclinic, $P2_1/n$
$a$ = 9.4764 (5) Å
$b$ = 8.2618 (5) Å
$c$ = 15.0990 (8) Å
$\beta$ = 106.259 (1)°
$V$ = 1134.85 (11) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.93 mm$^{-1}$
$T$ = 173 K
0.45 × 0.40 × 0.15 mm

### Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.477, $T_{max}$ = 0.761
5917 measured reflections
2428 independent reflections
2153 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.072
$S$ = 1.03
2428 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.9683 (14) | Cu1—O4$^{iii}$ | 1.9584 (14) |
| Cu1—O2$^{i}$ | 1.9716 (14) | Cu1—O5 | 2.1646 (15) |
| Cu1—O3$^{ii}$ | 1.9695 (13) | | |

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 2010).

We thank Hunan Medical Technical Secondary School and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5027).

## References

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# supporting information

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## *catena*-Poly[bis($\mu_4$-adipato-1:2:1′:2′$\kappa^4O^1$:$O^{1'}$:$O^4$:$O^{4'}$)bis(*N*,*N*-dimethylformamide)-1$\kappa O$,2$\kappa O$-dicopper(II)]

**Guo-Yun Wu and Seik Weng Ng**

### S1. Comment

Copper adipate furnishes a number of adducts with oxygen- and nitrogen-donor ligands. The parent compound itself exists as dihydrate, with the copper atom in a square-planar environment (Bakalbassis *et al.*, 2001; Zheng *et al.*, 2001). The four-coordinate nature explains the ability of the compound to expand the coordination number of the metal atom. In the present study, the DMF solvent used in the synthesis functions as donor ligand. The DMF adduct is formally the dicopper diadipate bis-adduct (Scheme I). The carboxyl $–CO_2$ ends of the approximately *U*-shape adipate dianion of polymeric $Cu_2(C_6H_8O_4)_2(C_3H_7NO)_2$ each bridges a pair of inversion-related, DMF-coordinated copper atoms (Fig. 1) to generate a ribbon motif that runs along the *b*-axis of the monoclinic unit cell. The geometry of the copper atom is a square pyramid; the apical site is occupied by the O atom of the DMF molecule whereas the four basal sites are occupied by the O atoms of the carboxyl ends.

### S2. Experimental

(1*H*-Benzimidazol-2-yl)-methanol (0.074 g, 0.5 mmol) was dissolved in a methanol/DMF mixture (*v*/*v* 1:1, 20 ml) and to this was added copper nitrate trihydrate (0.241 g, 1 mmol) followed by adipic acid (0.073 g, 0.5 mmol). The mixture was filtered and then set aside. Blue crystals were isolated after two weeks.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C).

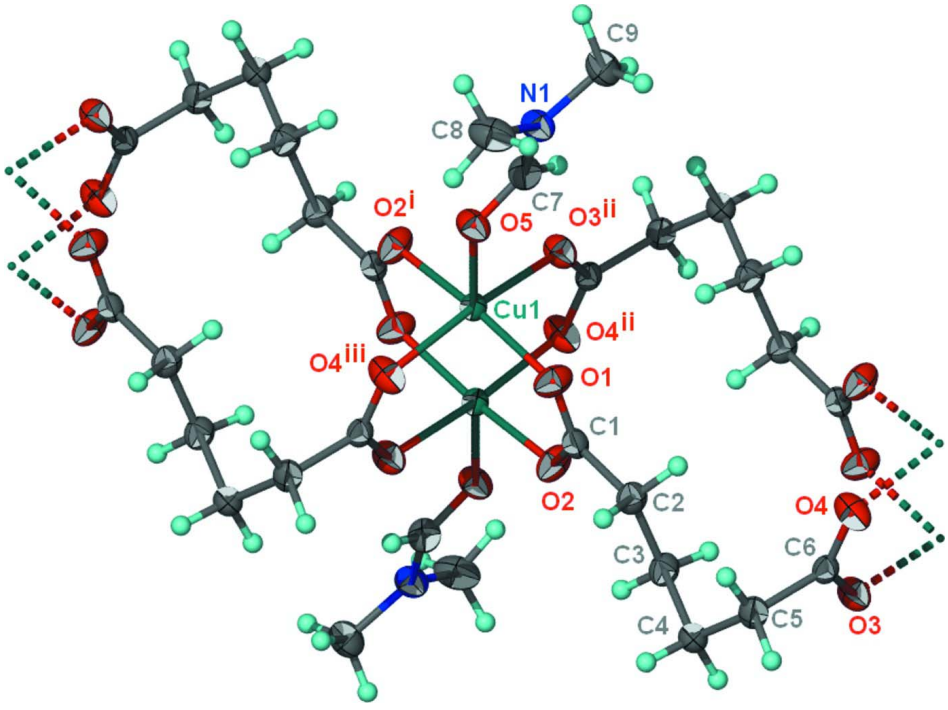


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of a portion of the ribbon structure of $Cu_2(C_6H_8O_4)_2(C_3H_7NO)_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

***catena*-Poly[bis($\mu_4$-adipato- 1:2:1′:2′$\kappa^4O^1$:$O^{1'}$:$O^4$:$O^{4'}$) bis(*N*,*N*-dimethylformamide)-1$\kappa O$,2$\kappa O$-dicopper(II)]**

*Crystal data*

$[Cu_2(C_6H_8O_4)_2(C_3H_7NO)_2]$
$M_r$ = 561.52
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 9.4764 (5) Å
$b$ = 8.2618 (5) Å
$c$ = 15.0990 (8) Å
$\beta$ = 106.259 (1)°
$V$ = 1134.85 (11) Å$^3$
$Z$ = 2
$F(000)$ = 580
$D_x$ = 1.643 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4192 reflections
$\theta$ = 2.3–27.0°
$\mu$ = 1.93 mm$^{-1}$
$T$ = 173 K
Block, blue
0.45 × 0.40 × 0.15 mm

*Data collection*

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.477, $T_{max}$ = 0.761
5917 measured reflections
2428 independent reflections
2153 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.3°
$h$ = −9→12
$k$ = −10→10
$l$ = −19→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.072$
$S = 1.03$
2428 reflections
147 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 1.1165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å$^{-3}$
$\Delta\rho_{min} = -0.23$ e Å$^{-3}$

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.43225 (2) | −0.00484 (2) | 0.564117 (15) | 0.01597 (9) |
| O1 | 0.52755 (16) | 0.20568 (17) | 0.60153 (10) | 0.0269 (3) |
| O2 | 0.64565 (17) | 0.21315 (17) | 0.49265 (10) | 0.0266 (3) |
| O3 | 0.72585 (15) | 0.89246 (17) | 0.52815 (9) | 0.0242 (3) |
| O4 | 0.60808 (16) | 0.88250 (19) | 0.63743 (10) | 0.0282 (3) |
| O5 | 0.31493 (16) | −0.01217 (17) | 0.66816 (10) | 0.0240 (3) |
| N1 | 0.12143 (18) | 0.0799 (2) | 0.71426 (11) | 0.0231 (3) |
| C1 | 0.6147 (2) | 0.2692 (2) | 0.56190 (13) | 0.0192 (4) |
| C2 | 0.6893 (2) | 0.4247 (2) | 0.60485 (14) | 0.0217 (4) |
| H2A | 0.7516 | 0.3998 | 0.6678 | 0.026* |
| H2B | 0.6124 | 0.5015 | 0.6110 | 0.026* |
| C3 | 0.7844 (2) | 0.5086 (2) | 0.55190 (14) | 0.0221 (4) |
| H3A | 0.7201 | 0.5715 | 0.5004 | 0.027* |
| H3B | 0.8351 | 0.4253 | 0.5249 | 0.027* |
| C4 | 0.8997 (2) | 0.6224 (2) | 0.61229 (14) | 0.0230 (4) |
| H4A | 0.9740 | 0.5566 | 0.6569 | 0.028* |
| H4B | 0.9504 | 0.6802 | 0.5726 | 0.028* |
| C5 | 0.8366 (2) | 0.7468 (2) | 0.66538 (13) | 0.0218 (4) |
| H5A | 0.7991 | 0.6896 | 0.7118 | 0.026* |
| H5B | 0.9167 | 0.8196 | 0.6990 | 0.026* |
| C6 | 0.7139 (2) | 0.8484 (2) | 0.60538 (12) | 0.0176 (4) |
| C7 | 0.1952 (2) | 0.0576 (2) | 0.65288 (14) | 0.0238 (4) |
| H7 | 0.1530 | 0.0984 | 0.5924 | 0.029* |
| C8 | 0.1795 (3) | 0.0257 (3) | 0.80898 (15) | 0.0324 (5) |
| H8A | 0.2752 | −0.0261 | 0.8166 | 0.049* |
| H8B | 0.1114 | −0.0523 | 0.8236 | 0.049* |
| H8C | 0.1911 | 0.1187 | 0.8506 | 0.049* |
| C9 | −0.0149 (2) | 0.1724 (3) | 0.69183 (16) | 0.0311 (5) |
| H9A | −0.0436 | 0.1998 | 0.6261 | 0.047* |
| H9B | −0.0003 | 0.2720 | 0.7285 | 0.047* |
| H9C | −0.0925 | 0.1074 | 0.7058 | 0.047* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.01828 (14) | 0.01576 (14) | 0.01519 (13) | 0.00059 (8) | 0.00683 (10) | −0.00014 (8) |
| O1 | 0.0302 (8) | 0.0256 (7) | 0.0286 (8) | −0.0089 (6) | 0.0143 (6) | −0.0088 (6) |
| O2 | 0.0381 (8) | 0.0200 (7) | 0.0264 (7) | −0.0063 (6) | 0.0169 (6) | −0.0056 (6) |
| O3 | 0.0232 (7) | 0.0299 (7) | 0.0204 (7) | 0.0058 (6) | 0.0075 (6) | 0.0064 (6) |
| O4 | 0.0275 (8) | 0.0383 (8) | 0.0212 (7) | 0.0110 (6) | 0.0111 (6) | 0.0085 (6) |
| O5 | 0.0225 (7) | 0.0303 (8) | 0.0215 (7) | 0.0058 (6) | 0.0100 (6) | 0.0036 (5) |
| N1 | 0.0221 (8) | 0.0269 (9) | 0.0225 (8) | 0.0027 (7) | 0.0099 (7) | 0.0002 (7) |
| C1 | 0.0186 (9) | 0.0169 (8) | 0.0206 (9) | 0.0030 (7) | 0.0032 (7) | 0.0001 (7) |
| C2 | 0.0244 (10) | 0.0186 (9) | 0.0230 (9) | −0.0008 (8) | 0.0082 (8) | −0.0039 (7) |
| C3 | 0.0262 (10) | 0.0187 (9) | 0.0227 (9) | −0.0004 (7) | 0.0089 (8) | −0.0017 (7) |
| C4 | 0.0190 (9) | 0.0205 (9) | 0.0300 (10) | 0.0017 (7) | 0.0074 (8) | 0.0024 (8) |
| C5 | 0.0215 (9) | 0.0191 (9) | 0.0214 (9) | −0.0002 (7) | 0.0003 (8) | −0.0002 (7) |
| C6 | 0.0186 (9) | 0.0144 (8) | 0.0184 (9) | −0.0013 (7) | 0.0030 (7) | −0.0015 (7) |
| C7 | 0.0282 (10) | 0.0250 (10) | 0.0213 (9) | 0.0016 (8) | 0.0122 (8) | 0.0024 (8) |
| C8 | 0.0252 (11) | 0.0518 (14) | 0.0216 (10) | 0.0005 (10) | 0.0092 (9) | 0.0013 (9) |
| C9 | 0.0284 (11) | 0.0294 (11) | 0.0387 (12) | 0.0063 (9) | 0.0150 (10) | −0.0017 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.9683 (14) | C2—H2B | 0.9900 |
| Cu1—O2$^{i}$ | 1.9716 (14) | C3—C4 | 1.533 (3) |
| Cu1—O3$^{ii}$ | 1.9695 (13) | C3—H3A | 0.9900 |
| Cu1—O4$^{iii}$ | 1.9584 (14) | C3—H3B | 0.9900 |
| Cu1—O5 | 2.1646 (15) | C4—C5 | 1.525 (3) |
| Cu1—Cu1$^{i}$ | 2.6069 (4) | C4—H4A | 0.9900 |
| O1—C1 | 1.262 (2) | C4—H4B | 0.9900 |
| O2—C1 | 1.251 (2) | C5—C6 | 1.512 (3) |
| O3—C6 | 1.256 (2) | C5—H5A | 0.9900 |
| O4—C6 | 1.262 (2) | C5—H5B | 0.9900 |
| O5—C7 | 1.235 (3) | C7—H7 | 0.9500 |
| N1—C7 | 1.321 (3) | C8—H8A | 0.9800 |
| N1—C8 | 1.452 (3) | C8—H8B | 0.9800 |
| N1—C9 | 1.457 (3) | C8—H8C | 0.9800 |
| C1—C2 | 1.521 (3) | C9—H9A | 0.9800 |
| C2—C3 | 1.529 (3) | C9—H9B | 0.9800 |
| C2—H2A | 0.9900 | C9—H9C | 0.9800 |
| | | | |
| O4$^{iii}$—Cu1—O1 | 90.48 (7) | C4—C3—H3A | 108.9 |
| O4$^{iii}$—Cu1—O3$^{ii}$ | 169.19 (6) | C2—C3—H3B | 108.9 |
| O1—Cu1—O3$^{ii}$ | 89.05 (6) | C4—C3—H3B | 108.9 |
| O4$^{iii}$—Cu1—O2$^{i}$ | 89.23 (7) | H3A—C3—H3B | 107.8 |
| O1—Cu1—O2$^{i}$ | 169.11 (6) | C5—C4—C3 | 114.04 (16) |
| O3$^{ii}$—Cu1—O2$^{i}$ | 89.19 (6) | C5—C4—H4A | 108.7 |
| O4$^{iii}$—Cu1—O5 | 96.03 (6) | C3—C4—H4A | 108.7 |
| O1—Cu1—O5 | 95.97 (6) | C5—C4—H4B | 108.7 |

| | | | |
|---|---|---|---|
| O3$^{ii}$—Cu1—O5 | 94.76 (6) | C3—C4—H4B | 108.7 |
| O2$^{i}$—Cu1—O5 | 94.88 (6) | H4A—C4—H4B | 107.6 |
| O4$^{iii}$—Cu1—Cu1$^{i}$ | 85.20 (4) | C6—C5—C4 | 114.07 (16) |
| O1—Cu1—Cu1$^{i}$ | 84.51 (4) | C6—C5—H5A | 108.7 |
| O3$^{ii}$—Cu1—Cu1$^{i}$ | 84.00 (4) | C4—C5—H5A | 108.7 |
| O2$^{i}$—Cu1—Cu1$^{i}$ | 84.62 (4) | C6—C5—H5B | 108.7 |
| O5—Cu1—Cu1$^{i}$ | 178.67 (4) | C4—C5—H5B | 108.7 |
| C1—O1—Cu1 | 122.68 (12) | H5A—C5—H5B | 107.6 |
| C1—O2—Cu1$^{i}$ | 122.64 (13) | O3—C6—O4 | 125.38 (18) |
| C6—O3—Cu1$^{ii}$ | 123.01 (13) | O3—C6—C5 | 117.60 (17) |
| C6—O4—Cu1$^{iv}$ | 122.10 (12) | O4—C6—C5 | 117.02 (16) |
| C7—O5—Cu1 | 118.87 (13) | O5—C7—N1 | 124.96 (19) |
| C7—N1—C8 | 121.24 (17) | O5—C7—H7 | 117.5 |
| C7—N1—C9 | 121.29 (18) | N1—C7—H7 | 117.5 |
| C8—N1—C9 | 117.24 (17) | N1—C8—H8A | 109.5 |
| O2—C1—O1 | 125.47 (18) | N1—C8—H8B | 109.5 |
| O2—C1—C2 | 118.63 (17) | H8A—C8—H8B | 109.5 |
| O1—C1—C2 | 115.89 (16) | N1—C8—H8C | 109.5 |
| C1—C2—C3 | 115.59 (16) | H8A—C8—H8C | 109.5 |
| C1—C2—H2A | 108.4 | H8B—C8—H8C | 109.5 |
| C3—C2—H2A | 108.4 | N1—C9—H9A | 109.5 |
| C1—C2—H2B | 108.4 | N1—C9—H9B | 109.5 |
| C3—C2—H2B | 108.4 | H9A—C9—H9B | 109.5 |
| H2A—C2—H2B | 107.4 | N1—C9—H9C | 109.5 |
| C2—C3—C4 | 113.16 (16) | H9A—C9—H9C | 109.5 |
| C2—C3—H3A | 108.9 | H9B—C9—H9C | 109.5 |

| | | | |
|---|---|---|---|
| O4$^{iii}$—Cu1—O1—C1 | 82.83 (16) | O1—C1—C2—C3 | −175.00 (17) |
| O3$^{ii}$—Cu1—O1—C1 | −86.36 (16) | C1—C2—C3—C4 | −158.25 (16) |
| O2$^{i}$—Cu1—O1—C1 | −5.6 (4) | C2—C3—C4—C5 | −53.1 (2) |
| O5—Cu1—O1—C1 | 178.95 (15) | C3—C4—C5—C6 | −54.7 (2) |
| Cu1$^{i}$—Cu1—O1—C1 | −2.30 (15) | Cu1$^{ii}$—O3—C6—O4 | −7.1 (3) |
| O4$^{iii}$—Cu1—O5—C7 | 175.47 (15) | Cu1$^{ii}$—O3—C6—C5 | 173.25 (12) |
| O1—Cu1—O5—C7 | 84.35 (16) | Cu1$^{iv}$—O4—C6—O3 | 6.2 (3) |
| O3$^{ii}$—Cu1—O5—C7 | −5.19 (16) | Cu1$^{iv}$—O4—C6—C5 | −174.09 (12) |
| O2$^{i}$—Cu1—O5—C7 | −94.78 (16) | C4—C5—C6—O3 | −38.7 (2) |
| Cu1$^{i}$—O2—C1—O1 | −2.9 (3) | C4—C5—C6—O4 | 141.63 (18) |
| Cu1$^{i}$—O2—C1—C2 | 175.51 (12) | Cu1—O5—C7—N1 | −171.07 (16) |
| Cu1—O1—C1—O2 | 3.8 (3) | C8—N1—C7—O5 | 1.7 (3) |
| Cu1—O1—C1—C2 | −174.68 (12) | C9—N1—C7—O5 | 176.2 (2) |
| O2—C1—C2—C3 | 6.4 (3) | | |

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) *x*, *y*+1, *z*.