# Refinement of the crystal structure of five ternary arsenides, $YCuAs_2$, $TbCuAs_2$, $DyCuAs_2$, $ErCuAs_2$ and $TmCuAs_2$

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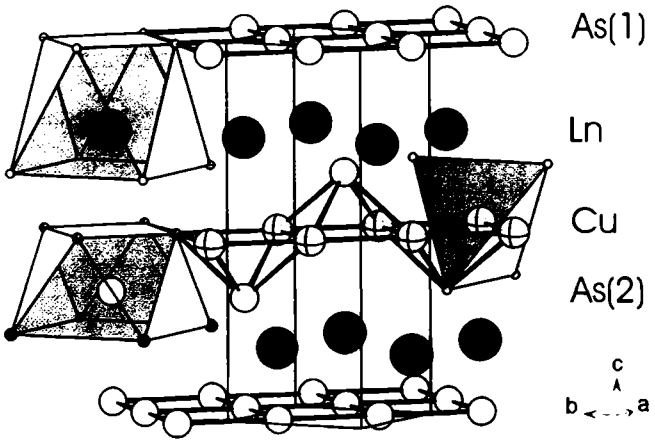
Received July 3, 2002, accepted and available on-line September 25, 2002; CSD-No. 412550, 412551, 412552, 412553 and 412554




**Abstract**

$As_2CuY$, tetragonal, *P4/nmm* (No. 129), $a = 3.888(1)$ Å, $c = 9.881(2)$ Å, $V = 149.4$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.031$, $wR_{ref}(F^2) = 0.062$, $T = 293$ K.

$As_2CuEr$, tetragonal, *P4/nmm* (No. 129), $a = 3.865(1)$ Å, $c = 9.802(2)$ Å, $V = 146.4$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.031$, $wR_{ref}(F^2) = 0.068$, $T = 293$ K.

$As_2CuTb$, tetragonal, *P4/nmm* (No. 129), $a = 3.901(1)$ Å, $c = 9.901(2)$ Å, $V = 150.7$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.024$, $wR_{ref}(F^2) = 0.054$, $T = 293$ K.

$As_2CuTm$, tetragonal, *P4/nmm* (No. 129), $a = 3.854(1)$ Å, $c = 9.778(3)$ Å, $V = 145.2$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.028$, $wR_{ref}(F^2) = 0.065$, $T = 295$ K.

$As_2CuDy$, tetragonal, *P4/nmm* (No. 129), $a = 3.884(1)$ Å, $c = 9.847(2)$ Å, $V = 148.5$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.031$, $wR_{ref}(F^2) = 0.065$, $T = 295$ K.

**Source of material**

Grey rod or platelet shaped single crystals of the compounds $LnCuAs_2$ (Ln = Y, Tb, Dy, Er and Tm) are prepared by reaction of stoichiometric amounts of the elements in a LiCl/KCl flux (1123 K; 6 days) in quartz ampoules. The flux is removed with water and ethanol after cooling, and the crystals are allowed to dry in air. EDX analyses reveal no detectable impurities from flux or other elements.

**Discussion**

The existence of the ternary rare-earth element copper arsenides $LnCuAs_2$ (Ln = Y, La-Lu, except Eu and Pm) has been confirmed by X-ray powder measurements [1]. Single crystal investigations on selected examples corroborated, that all stoichiometric compounds $LnCu_{1+x}As_2$ ($x = 0$) adopt the $HfCuSi_2$ type [3-5], whereas the non-stoichiometric compounds (compounds with $x > 0$) crystallize in a stuffed variant of this structure type [2,5]. $LaCu_{1.23}As_2$, as an exception, crystallizes in a stuffed variant of the $SrZnBi_2$ type [2]. We report the results of the single crystal investigations of $YCuAs_2$, $TbCuAs_2$, $DyCuAs_2$, $ErCuAs_2$ and $TmCuAs_2$, all adopting the $HfCuSi_2$ type. The structure of the title compounds contains puckered double As/Cu sheets consisting of tetragonal $AsCu_4$-pyramids, linked via common edges, and planar square nets of As. Double sheets and planar layers are separated by layers of the Ln atoms.

## 1. Yttrium copper diarsenide, $YCuAs_2$

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | grey rod, size 0.01 × 0.06 × 0.20 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| $\mu$: | 480.96 cm$^{-1}$ |
| Diffractometer, scan mode: | Stoe-IPDS, $\varphi$ |
| $2\theta_{max}$: | 56° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1889, 141 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 113 |
| $N(param)_{refined}$: | 12 |
| Programs: | SHELXL-97 [6], DIAMOND [7] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Y | 2c | 1/4 | 1/4 | 0.2376(2) | 0.0072(6) | $U_{11}$ | 0.0111(9) | 0 | 0 | 0 |
| As(1) | 2a | 3/4 | 1/4 | 0 | 0.0148(6) | $U_{11}$ | 0.0087(9) | 0 | 0 | 0 |
| As(2) | 2c | 3/4 | 3/4 | 0.3391(2) | 0.0076(5) | $U_{11}$ | 0.010(1) | 0 | 0 | 0 |
| Cu | 2b | 3/4 | 1/4 | 1/2 | 0.0110(6) | $U_{11}$ | 0.013(1) | 0 | 0 | 0 |

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## 2. Terbium copper diarsenide, TbCuAs2

**Table 3.** Data collection and handling.

| | |
|---|---|
| Crystal: | grey platelet, size 0.01 × 0.19 × 0.30 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| $\mu$: | 517.95 $cm^{-1}$ |
| Diffractometer, scan mode: | Stoe-IPDS, $\varphi$ |
| $2\theta_{max}$: | 51.28° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1090, 115 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 104 |
| $N(param)_{refined}$: | 12 |
| Programs: | SHELXL-97 [6], DIAMOND [7] |

**Table 4.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Tb | 2*c* | 1/4 | 1/4 | 0.23803(8) | 0.0059(4) | $U_{11}$ | 0.0149(5) | 0 | 0 | 0 |
| As(1) | 2*a* | 3/4 | 1/4 | 0 | 0.0124(7) | $U_{11}$ | 0.015(1) | 0 | 0 | 0 |
| As(2) | 2*c* | 3/4 | 3/4 | 0.3401(2) | 0.0049(6) | $U_{11}$ | 0.017(1) | 0 | 0 | 0 |
| Cu | 2*b* | 3/4 | 1/4 | 1/2 | 0.0102(8) | $U_{11}$ | 0.016(1) | 0 | 0 | 0 |

## 3. Dysprosium copper diarsenide, DyCuAs2

**Table 5.** Data collection and handling.

| | |
|---|---|
| Crystal: | grey platelet, size 0.01 × 0.14 × 0.24 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| $\mu$: | 538.82 $cm^{-1}$ |
| Diffractometer, scan mode: | Stoe-IPDS, $\varphi$ |
| $2\theta_{max}$: | 56.08° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1623, 138 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 123 |
| $N(param)_{refined}$: | 12 |
| Programs: | SHELXL-97 [6], DIAMOND [7] |

**Table 6.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Dy | 2*c* | 1/4 | 1/4 | 0.23753(9) | 0.0058(4) | $U_{11}$ | 0.0083(5) | 0 | 0 | 0 |
| As(1) | 2*a* | 3/4 | 1/4 | 0 | 0.0126(8) | $U_{11}$ | 0.007(1) | 0 | 0 | 0 |
| As(2) | 2*c* | 3/4 | 3/4 | 0.3390(2) | 0.0053(7) | $U_{11}$ | 0.010(1) | 0 | 0 | 0 |
| Cu | 2*b* | 3/4 | 1/4 | 1/2 | 0.010(1) | $U_{11}$ | 0.011(1) | 0 | 0 | 0 |

## 4. Erbium copper diarsenide, ErCuAs2

**Table 7.** Data collection and handling.

| | |
|---|---|
| Crystal: | grey platelet, size 0.02 × 0.11 × 0.38 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71069 Å) |
| $\mu$: | 578.05 $cm^{-1}$ |
| Diffractometer, scan mode: | Stoe-IPDS, $\varphi$ |
| $2\theta_{max}$: | 52.26° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1132, 117 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 111 |
| $N(param)_{refined}$: | 12 |
| Programs: | SHELXL-97 [6], DIAMOND [7] |

**Table 8.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Er | 2*c* | 1/4 | 1/4 | 0.23673(8) | 0.0078(5) | $U_{11}$ | 0.0094(6) | 0 | 0 | 0 |
| As(1) | 2*a* | 3/4 | 1/4 | 0 | 0.0127(7) | $U_{11}$ | 0.008(1) | 0 | 0 | 0 |
| As(2) | 2*c* | 3/4 | 3/4 | 0.3368(2) | 0.0069(7) | $U_{11}$ | 0.010(1) | 0 | 0 | 0 |
| Cu | 2*b* | 3/4 | 1/4 | 1/2 | 0.0109(8) | $U_{11}$ | 0.011(1) | 0 | 0 | 0 |

## 5. Thulium copper diarsenide, $TmCuAs_2$

**Table 9.** Data collection and handling.

| | |
|---|---|
| Crystal: | grey platelet, size 0.01 × 0.22 × 0.51 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 599.61 $cm^{-1}$ |
| Diffractometer, scan mode: | Stoe-IPDS, $\varphi$ |
| $2\theta_{max}$: | 56.32° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1747, 135 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 125 |
| $N(param)_{refined}$: | 12 |
| Programs: | SHELXL-97 [6], DIAMOND [7] |

**Table 10.** Atomic coordinates and displacement parameters (in $Å^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Tm | 2*c* | 1/4 | 1/4 | 0.23632(8) | 0.0083(4) | $U_{11}$ | 0.0057(5) | 0 | 0 | 0 |
| As(1) | 2*a* | 3/4 | 1/4 | 0 | 0.0127(6) | $U_{11}$ | 0.004(1) | 0 | 0 | 0 |
| As(2) | 2*c* | 3/4 | 3/4 | 0.3357(2) | 0.0076(6) | $U_{11}$ | 0.005(1) | 0 | 0 | 0 |
| Cu | 2*b* | 3/4 | 1/4 | 1/2 | 0.0116(7) | $U_{11}$ | 0.006(1) | 0 | 0 | 0 |

*Acknowledgments.* The authors thank the Deutsche Forschungsgemeinschaft and the Fonds der Chemischen Industrie for financial support.

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