

# Study on the Crystal of Daomanite

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**Abstract:** It was not possible to carry out a complete analyses of crystal, as the experiment by Ding and Shi et al.. It's analysis precision  $R=0.25$  or more big than this, which value are not satisfied for single crystal study, but we through many test and found the best:  $[R(\text{int})=14.5\%]$ . The final full-matrix least-squares refinement on  $F^2$  converged to  $R_1=0.0791$  and  $wR_2=0.1864$  for 704 observed reflections  $[I \geq 2\sigma(I)]$ . Daomanite is orthorhombic system, space group  $Cmc2_1$ ,  $a=3.7520(8)\text{\AA}$ ,  $b=15.844(4)\text{\AA}$ ,  $c=5.8516(12)\text{\AA}$ ,  $\alpha=\beta=\gamma=90^\circ$ .  $V=347.86(14)\text{\AA}^3$ ,  $Z=4$ . Daomanite chemical formula is  $\text{CuPtAsS}_2$ . Idealized composition  $\text{Me}^+\text{M}^{2+}\text{M}^{2+}\text{S}_2=\text{CuS}\cdot\text{PtAsS}$ . There is no other similar mineral in the world.

**Key words:** daomanite,  $\text{CuPtAsS}_2$  new mineral species, Yanshan Mountains, Chengde, China

## 1 Geological Setting and Occurrence

Daomanite was found at the Sandaogou copper deposit, Luanping county, Chengde city (Prefecture), Hebei Province, China (lat.  $41^\circ49'$  N, long.  $116^\circ09'$  E). It is situated in contact between pyroxenite and anorthosite granite-gneiss. Ore zone is a few hundred metres long and a few metres thick. Daomanite (Yu et al., 1978) was found associated with lisiguangite. Daomanite widely distributed in the upper part of ore body, and lisiguangite in the lower part. The upper part is rich in copper and cobalt as well as carrollite and Co-malanite. The lower part is in precious metal such as PGE and Ag. Daomanite associated bornite, chalcopyrite, cooperite, galena and minimum minerals: damiaoite, yixunite (Yu, 1977) (Figs. 1, 2).

The upper and lower ore deposit was formed by a multistage hydrothermal process of a contact-metamorphic. The orebodies occur as an exoskarn. It is thus a mesothermal deposit.

## 2 Experiments

The low-temperature ( $113\pm2\text{K}$ ) single-crystal X-ray data were collected using monochromatic  $\text{MoK}\alpha$  radiation at 50kV and 16mA on a Rigaku Micro Max-007 VariMaxTM four-circle diffractometer equipped with a Rigaku Saturn 724+ detector.

Data collection was controlled using the Crystal Clear program (Rigaku, 2009). Computations were performed using the SHELXTL NT version 5.10 program (Sheldrick,



Fig. 1. Crystal habit of daomanite and its orange red clearages.

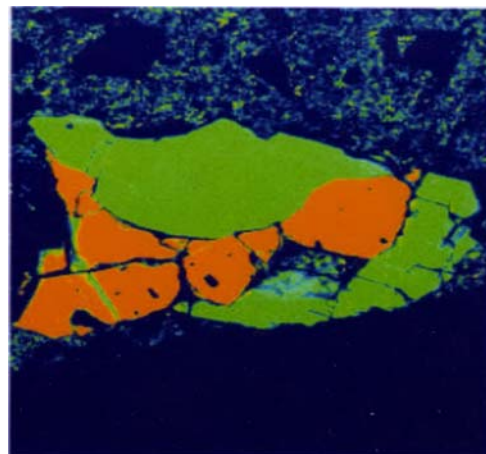


Fig. 2. Daomanite (brown) intimately associated with cooperite.

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**Table 1 Crystal data, data collection information and refinement details for Daomanite**

Refined formula	CuPtAsS <sub>2</sub>
Formula weight	397.67
Space Group	<i>Cmc</i> 2 <sub>1</sub>
<i>a</i> (Å)	3.7520(8)
<i>b</i> (Å)	15.844(4)
<i>c</i> (Å)	5.8516(12)
$\alpha=\beta=\gamma$ (°)	90
<i>V</i> (Å <sup>3</sup> ), <i>Z</i>	347.86(14), 4
Density (calc.) (g/cm <sup>3</sup> )	7.593
$\mu$ (mm <sup>-1</sup> )	56.648 mm <sup>-1</sup>
Crystal dimensions (mm)	0.14×0.12×0.04
<i>F</i> (000)	688
Diffractionmeter	Rigaku Micro MicroMax-007+VariMaxTM
$\lambda$ (MoK $\alpha$ )(A), T(K)	0.071073, 293(2)
Number of frames	540
Scan time (s/°)	10
$\theta$ range for collection (°)	2.57–25.01
Limiting indices	−4≤ <i>h</i> ≤4, −18≤ <i>k</i> ≤11, −6≤ <i>l</i> ≤6
Total reflections measured	2395
Unique reflections 3895/*	357 [R(int)=14.05%]
Reflections > 4 $\sigma$ ( <i>F</i> )	357
Refinement on	<i>F</i> <sup>2</sup>
<i>R</i> <sub>1</sub> ( <i>F</i> ), <i>wR</i> <sub>2</sub> ( <i>F</i> <sup>2</sup> )	7.91%, 18.64%
<i>R</i> <sub>1</sub> all ( <i>F</i> ), <i>wR</i> <sub>2</sub> all ( <i>F</i> <sup>2</sup> )	8.19%, 18.77%
Extinction Coefficient	0.0
No. of refined parameters	55
Goof on <i>F</i> <sup>2</sup>	1.007
$\Delta\rho_{\text{min}}, \Delta\rho_{\text{max}}$ (e/Å <sup>3</sup> )	−0.8234, 0.9893

**Table 2 Bond lengths (Å) and angles (°) for diomanite**

Pt(1)–S(1)	2.40(2)	S(1)–Pt(1)–S(2)	89.8(6)
Pt(1)–As(1) #1	2.441(5)	As(1) #1–Pt(1)–S(2)	80.2(3)
Pt(1)–As(1) #2	2.441(5)	As(1) #2–Pt(1)–S(2)	179.3(4)
Pt(1)–As(1) #3	2.461(11)	As(1) #3–Pt(1)–S(2)	88.2(6)
Pt(1)–S(2) #4	2.465(12)	S(2) #4–Pt(1)–S(2)	99.1(7)
Pt(1)–S(2)	2.465(12)	S(1)–As(1)–Pt(1) #5	108.7(3)
As(1)–S(1)	2.280(19)	S(1)–As(1)–Pt(1) #6	108.7(3)
As(1)–Pt(1) #5	2.441(5)	Pt(1) #5–As(1)–Pt(1) #6	100.5(3)
As(1)–Pt(1) #6	2.441(5)	S(1)–As(1)–Pt(1) #7	105.7(5)
As(1)–Pt(1) #7	2.461(11)	Pt(1) #5–As(1)–Pt(1) #7	116.5(3)
Cu(1)–s(2) #8	2.24(2)	Cu(1) #6–As(1)–Pt(1) #7	116.5(3)
Cu(1)–S(2) #8	2.24(2)	Pt(1) #6–As(1)–Pt(1) #7	116.5(3)
S(2)–Cu(1) #7	2.27(3)	S(2) #8–Cu(1)–S(2) #7	123.7(10)
Cu(1)–S(2) #9	2.314(3)	S(2) #8–Cu(1)–S(1) #9	108.8(7)
Cu(1)–S(1)	2.314(14)	S(2) #7–Cu(1)–S(1) #9	103.2(6)
S(1)–Cu(1) #4	2.314(14)	S(2) #8–Cu(1)–S(1)	108.8(7)
S(2)–Cu(1) #10	2.24(2)	S(2) #7–Cu(1)–S(1)	103.2(6)
S(2)–Cu(1) #3	2.27(3)	S(1) #9–Cu(1)–S(1)	108.4(10)
S(21)–Pt(1) #9	2.465(12)	As(1)–S(1)–Cu(1) #4	99.3(7)
		As(1)–S(1)–Cu(1)	99.3(7)
S(1)–Pt(1)–As#1	90.1(4)	Cu(1) #4–S(1)–Cu(1)	108.4(10)
S(1)–Pt(1)–As(1) #2	90.1(4)	As(1)–S(1)–Pt(1)	102.7(7)
As(1) #1–Pt(1)–As(1) #2	100.5(3)	Cu(1) #4–S(1)–Pt(1)	120.9(7)
S(1)–Pt(1)–As(1) #3	177.0(5)	Cu(1)–S(1)–Pt(1)	120.9(7)
As(1) #1–Pt(1)–As(1) #3	91.8(2)	Cu(1) #10–S(2)–Cu(1) #3	94.5(8)
As(1) #2–Pt(1)–As(1) #3	91.8(2)	Cu(1) #10–S(2)–Pt(1)	118.6(7)
S(1)–Pt(1)–S(2) #4	89.8(6)	Cu(1) #3–S(2)–Pt(1)	113.6(7)
As(1) #1–Pt(1)–S(2) #4	179.3(4)	Cu(1) #10–S(2)–Pt(1) #9	118.6(7)
As(1) #2–Pt(1)–S(2) #4	80.2(3)	Cu(1) #3–S(2)–Pt(1) #9	113.6(7)
As(1) #3–Pt(1)–S(2) #4	88.2(6)	Pt(1)–S(2)–Pt(1) #9	99.1(7)

**Table 3 Atomic coordinates (×10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup>×10<sup>3</sup>) for R90705A**

	X	Y	Z	U(eq)	U11	U22	U33	U23	U13	U12
Pt(1)	0	1774(2)	7625(4)	11(1)	13(1)	16(1)	4(1)	−1(1)	0	0
As(1)	0	2323(5)	1559(18)	12(2)	13(2)	13(2)	11(2)	0(1)	0	0
Cu(1)	5000	487(5)	2460(20)	19(2)	22(4)	28(5)	7(5)	0(6)	0	0
S(1)	0	1165(11)	3870(40)	11(4)	12(4)	12(4)	11(4)	0(1)	0	0
S(1)	5000	848(11)	8710(40)	13(4)	13(4)	13(4)	13(4)	0(1)	0	0

Note: *U*(eq) is defined as one third of the trace of the orthogonalised *U*<sub>ij</sub> tensor. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12}]$ .

**Table 4 Hydrogen coordinates (×10<sup>4</sup>) and isotropic Displacement parameters (Å<sup>2</sup>×10<sup>3</sup>) for R90705A**

Pt(1) #5–As(1)–S(1)–Cu(1) #4	179.0(6)	As(1) #2–Pt(1)–S(1)–Cu(1) #4	−58.9(8)
Pt(1) #6–As(1)–S(1)–Cu(1) #4	70.5(6)	As(1) #3–Pt(1)–S(1)–Cu(1) #4	70.8(8)
Pt(1) #7–As(1)–S(1)–Cu(1) #4	−55.3(6)	S(2) #4–Pt(1)–S(1)–Cu(1) #4	21.3(8)
Pt(1) #5–As(1)–S(1)–Cu(1)	−70.5(6)	S(2)–Pt(1)–S(1)–Cu(1) #4	120.4(8)
Pt(1) #6–As(1)–S(1)–Cu(1)	−179.0(6)	As(1) #1–Pt(1)–S(1)–Cu(1)	58.9(8)
Pt(1) #7–As(1)–S(1)–Cu(1)	55.3(6)	As(1) #2–Pt(1)–S(1)–Cu(1)	159.4(8)
Pt(1) #5–As(1)–S(1)–Pt(1)	54.2(2)	As(1) #3–Pt(1)–S(1)–Cu(1)	−70.8(8)
Pt(1) #6–As(1)–S–Pt(1)	−54.2(2)	S(2) #4–Pt(1)–S(1)–Cu(1)	−120.4(8)
Pt(1) #7–As(1)–S(1)–Pt(1)	180.0	S(2)–Pt(1)–S(1)–Cu(1)	−21.3(8)
Pt(1) #7–As(1)–S(1)–Pt(1)	180.0	S(1)–Pt(1)–S(1)–Cu(1) #10	−39.5(10)
S(2) #8–Cu(1)–S(1)–As(1)	−165.0(8)	As(1) #1–Pt(1)–S(2)–Cu(1) #10	−129.6(9)
S(2) #7–Cu(1)–S(1)–As(1)	−32.1(7)	As(1) #2–Pt(1)–S(2)–Cu(1) #10	−44(61)
S(1) #9–Cu(1)–S(1)–As(1)	76.8(11)	As(1) #3–Pt(1)–S(2)–Cu(1) #10	138.2(9)
S(2) #8–Cu(1)–S(1)–Cu(1) #4	−61.8(14)	S(2) #4–Pt(1)–S(2)–Cu(1) #10	50.3(15)
S(2) #7–Cu(1)–S(1)–Cu(1) #4	71.1(9)	S(1)–Pt(1)–S(2)–Cu(1) #3	−149.0(7)
S(1) #9–Cu(1)–S(1)–Cu(1) #4	180.001(1)	As(1) #1–Pt(1)–S(2)–Cu(1) #3	120.8(6)
S(2) #8–Cu(1)–S(1)–Pt(1)	84.0(10)	As(1) #2–Pt(1)–S(2)–Cu(1) #3	−66(61)
S(2) #7–Cu(1)–S(1)–Pt(1)	−143.0(8)	As(1) #3–Pt(1)–S(2)–Cu(1) #3	28.7(6)
S(1) #9–Cu(1)–S(1)–Pt(1)	−34.1(15)	S(2) #4–Pt(1)–S(2)–Cu(1) #3	−59.2(11)
As(1) #1–Pt(1)–S(1)–As(1)	−50.23(15)	S(1)–Pt(1)–S(2)–Pt(1) #9	90.2(7)
As(1) #2–Pt(1)–S(1)–As(1)	50.23(15)	As(1) #1–Pt(1)–S(2)–Pt(1) #9	0.1(7)
As(1) #3–Pt(1)–S(1)–As(1)	180.00(3)	As(1) #2–Pt(1)–S(2)–Pt(1) #9	173(60)
S(2) #4–Pt(1)–S(1)–As(1)	130.4(3)	As(1) #3–Pt(1)–S(2)–Pt(1) #9	−92.1(7)
S(2)–Pt(1)–S(1)–As(1)	−130.4(3)	S(2) #4–Pt(1)–S(2)–Pt(1) #9	180
As(1) #1–Pt(1)–S(1)–Cu(1) #4	−159.4(8)		

1997). Analytical expressions of atomic scattering factors were employed, and anomalous dispersion corrections were incorporated (Prince, 1992) (Tables 1, 2, 3, 4)

The crystal structure was determined by direct methods using SHELXS-86 (Sheldrick, 1986) and subsequent

Fourier and Fourier-difference syntheses using SHELXS-93 (Sheldrick, 1993). After the determination of all atom positions, the displacement parameters for non-hydrogen atoms were refined with anisotropic thermal parameters, whereas hydrogen atoms were refined isotropically.

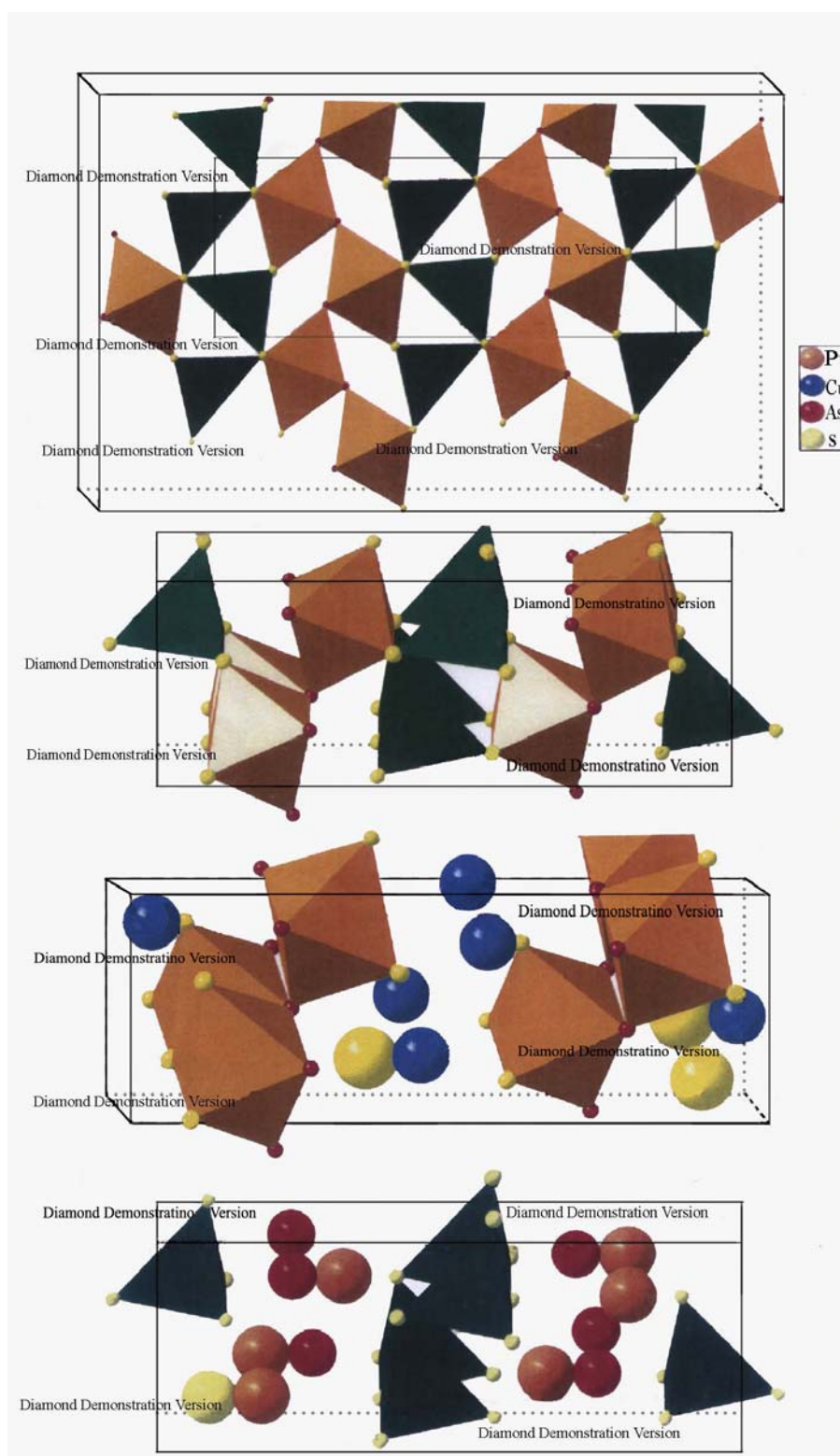


Fig. 3. Accumulation structure map of daomanites.

Refinement on  $F^2$  was carried out by full-matrix least squares (SHELXL-93).

Unit-cell data were refined with 1761 reflections with  $3.0^\circ < 2\theta < 25.1^\circ$ . No decay was observed in data collection. Raw intensities were corrected for Lorentz and polarization effects, and for absorption by empirical method. Direct phase determination yielded the positions of all non-hydrogen atoms. All non-hydrogen atoms were subjected to anisotropic refinement.

### 3 Structure of Daomanite

The three Pt in Daomanite are coordinated three S form an octahedron, the one S united As form (As,S) ion group, coordinated Cu form three distorted tetrahedron Cu(As,S)<sub>2</sub> (Fig. 3).

Utility of diamond software have drawn 4 structure maps of daomanite. The chemical composition of octahedral are PtAs<sub>3</sub>S<sub>3</sub>, tetrahedral are CuS<sub>4</sub> in Fig. 3. The octahedron linked each other form octahedron chains, parallel along an axis form octahedral chains. By sharing corners from octahedral chains are connected and form octahedral double chains are linked as shared edges. The octahedral chains are linked with Cu-S octahedrons as shared corners. Daomanite is a new chain mineral of arsenic sulphide.

### 4 Conclusions

Daomanite is orthorhombic system, space group  $Cmc2_1$ ,  $a=3.7520(8)\text{\AA}$ ,  $b=15.844(4)\text{\AA}$ ,  $c=5.8516(12)\text{\AA}$ ,  $\alpha=\beta=\gamma=90^\circ$ .  $V=347.86(14)\text{\AA}^3$ ,  $Z=4$ . Daomanite chemical formula is  $\text{CuPtAsS}_2$ . Idealized composition  $\text{Me}^+\text{M}^{2+}\text{M}^{2+}\text{S}_2 = \text{CuS}\cdot\text{PtAsS}$ . There is no other similar mineral in the world.

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