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Campigliaite, $Cu_4Mn(SO_4)_2(OH)_6 \cdot 4H_2O$, a new mineral from Campiglia Marittima, Tuscany, Italy

I. Occurrence and description

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Abstract

Campigliaite, a new copper and manganese sulfate mineral, occurs as tufts of light blue crystals in the sulfide ore bodies of Temperino mine, Campiglia Marittima, Tuscany, Italy. It is monoclinic, space group $C2$, with $a = 21.707$, $b = 6.098$, $c = 11.245$Å, $\beta = 100.3°$. The tiny crystals, elongated [010] and flattened {100}, are always twinned (100). The calculated density is 3.06 g cm^{-3}. Optically it is biaxial (–) with $\alpha = 1.589$, $\beta = 1.645$, $\gamma = 1.659$. The strongest lines in the X-ray powder pattern are 10.68(100)(200), 5.34 (60)(400), 3.56 (44)(600), 2.673(5)(022 and 800).

The structure was solved using 689 independent reflections and refined to an R value of 0.124. The dominant structural feature is the arrangement of copper–oxygen polyhedra into dense sheets, parallel to (100). The sulfate groups are linked by a corner to both sides of sheets. The Mn atom coordinates four water molecules and two oxygen atoms of sulfate groups belonging to the same Cu–O–S layer. Subsequent layers are connected to each other by hydrogen bonds. The relationship between the structures of campigliaite and devillite and serpierite is discussed.

Introduction

In a previous paper (Conticini *et al.*, 1980) dealing with the alteration minerals from Campiglia Marittima (Tuscany, Italy) we briefly described a mineral, a hydrated basic sulfate of copper and manganese, which appeared to be different from any known sulfate. Further study revealed the mineral in question to be a new species.

The mineral, $Cu_4Mn(SO_4)_2(OH)_6 \cdot 4H_2O$, is named campigliaite for the locality. Both the mineral and the name have been approved by the Commission on New Minerals and Mineral Names, IMA. A type specimen is deposited in the mineralogical Museum of Florence University (regional collection #214/I).

On the basis of the ideal formula, cell parameters and crystal structure, campigliaite is related to the serpierite–devillite series and, if one extra molecule of H_2O is neglected, it can be considered the manganese analogue of devillite.

Occurrence and paragenesis

The geographic location of Campiglia Marittima is depicted in Figure 1. A brief account of the geology and ore deposits of the area is given in the above quoted paper, specially devoted to secondary minerals. The main tunnel of the third level of the "Miniera del Temperino" which goes from "Pozzo Earle" to "Pozzo Gowet" crosses through sulfide ore bodies (chalcopyrite, pyrite, sphalerite, galena, pyrrhotite, *etc.*). Starting from the point where the tunnel leaves the marbles and goes into the skarn, many copper oxysalts appear in the order: malachite, brochantite, antlerite, chalcanthite. This sequence is related to the increasing acidity of solutions and the increasing concentration of SO_4. Serpierite also is common and widespread in the tunnel. However the most common and widespread secondary mineral is gypsum which occurs both as transparent crystals and as incrustations on other minerals. It is interesting to note that when two or more copper sulfates are present together, one can observe antlerite often grown on brochantite and chalcanthite grown on antlerite.

Campigliaite was found only on the vugs of an ilvaite-rich skarn, collected in a side-tunnel ("galleria del fornello") of the main tunnel. It occurs as

0003–004X/82/0304–0385$02.00

Distante - angoli Cartesiane - Trasformata in coordinate polari

	ALPHA	BETA	GAMMA
	90.000	180.000	90.000
COSINE	0.000000	-0.100000	0.000000

	CR	ALPHAR	BETAR	GAMMAR
	0.000000	70.000	170.000	90.000
COSINE		-0.000000	0.173981	-0.000000

NO.	TRANSFORMED X	TRANSFORMED Y	TRANSFORMED Z
1	1.000000 1. X 0. Y 0. Z	0.000000 0. X 1. Y 0. Z	0.000000 0. X 0. Y 1. Z
2	1.000000 -1. X 0. Y 0. Z	0.000000 0. X 1. Y 0. Z	1.000000 0. X 0. Y -1. Z
3	0.500000 1. X 0. Y 0. Z	0.500000 0. X 1. Y 0. Z	0.000000 0. X 0. Y 1. Z
4	0.500000 -1. X 0. Y 0. Z	0.500000 0. X 1. Y 0. Z	1.000000 0. X 0. Y -1. Z

NO.	AT-	X	Y	Z	B11	B22	B33	B12	B13	B23	MAT
1	B01	0.000000	0.500000	-0.000100	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
2	B02	0.129000	0.750000	0.251100	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
3	B03	0.259400	1.250000	0.255400	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
4	B04	0.129700	0.518000	0.501300	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
5	B05	0.388100	0.437000	0.261200	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
6	B06	0.112400	0.201000	0.055600	0.700000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
7	B07	0.378000	0.701000	0.486000	0.700000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
8	B08	0.308700	0.023000	0.167000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
9	B09	0.121000	0.541000	0.167000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
10	B10	0.101000	0.237000	0.074000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
11	B11	0.195000	0.736000	0.061000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
12	B12	0.294000	0.255000	0.459000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
13	B13	0.337000	0.755000	0.445000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
14	B14	0.218000	0.024000	0.311000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
15	B15	0.215000	0.578000	0.316000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
16	B16	0.057000	0.104000	-0.065000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
17	B17	0.103000	0.033000	0.145000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
18	B11	0.203000	0.416000	0.069000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
19	B12	0.402000	0.818000	0.570000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
20	B13	0.416000	0.586000	0.372000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
21	B14	0.423000	0.914000	0.520000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
22	B15	0.500000	0.789000	0.236000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
23	B16	0.573000	0.118000	0.277000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
24	B17	0.471000	0.159000	0.356000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
25	B18	0.434000	0.167000	0.110000	1.500000	0.000000	0.000000	0.000000	0.000000	0.000000	1.
26	CELL	0.000000	0.000000	0.000000	0.010000	0.000000	0.000000	0.000000	0.000000	0.000000	2.
27	GRID	0.500000	0.500000	0.500000	0.010000	0.000000	0.000000	0.000000	0.000000	0.000000	2.

[illegible]

WITH RADIUS OR. IF A BOX, WITH SEMIDIMENSION
A B C

[illegible] 2.900 0.000 0.000

VECTORS FROM ATOM (1.55501.) TO ATOMS 8 THROUGH 25

CU1	[illegible]	(1.55501.) 0.2488 0.5200-0.0003	(9.55501.) 0.2910 0.5410 0.1670	D = [illegible]
CU1	[illegible]		(11.55501.) 0.1950 0.7360 0.0610	D = [illegible]
CU1	[illegible]		(8.55404.) 0.1940 0.5270-0.1870	D = [illegible]
CU1	[illegible]		(11.54404.) 0.3050 0.2360-0.0610	D = [illegible]
CU1	[illegible]		(10.55404.) 0.3190 0.7670-0.0740	D = [illegible]
CU1	[illegible]		(10.55501.) 0.1910 0.2670 0.0740	D = [illegible]

VECTORS FROM ATOM (2.55501.) TO ATOMS 8 THROUGH 25

CU2	O5	(2.55501.) 0.2570 0.7800 0.2511	(15.55501.) 0.2180 0.5580 0.3160	D = [illegible]
CU2	[illegible]		(14.56501.) 0.2190 1.0260 0.3110	D = [illegible]
CU2	[illegible]		(9.55501.) 0.2710 0.5410 0.1620	D = [illegible]
CU2	[illegible]		(8.56501.) 0.3060 1.0230 0.1870	D = [illegible]
CU2	O4		(11.55501.) 0.1950 0.7360 0.0610	D = [illegible]
CU2	[illegible]		(13.55501.) 0.3270 0.7550 0.4450	D = [illegible]

VECTORS FROM ATOM (3.55501.) TO ATOMS 8 THROUGH 25

CU3	O7	(3.55501.) 0.2596 0.2590 0.2554	(14.55501.) 0.2190 0.0260 0.3110	D = 1.940
CU3	O1		(8.55501.) 0.3060 0.0230 0.1870	D = 1.990
CU3	O2		(9.55501.) 0.2910 0.5410 0.1670	D = 2.168
CU3	O8		(15.55501.) 0.2180 0.5580 0.3160	D = 2.208
CU3	O5		(12.55501.) 0.2960 0.2550 0.4520	D = 2.278
CU3	O3		(10.55501.) 0.1810 0.2670 0.0740	D = 2.406

VECTORS FROM ATOM (4.55501.) TO ATOMS 8 THROUGH 25

CU4	O5	(4.55501.) 0.2497 0.5180 0.5013	(12.55504.) 0.2040 0.7550 0.5410	D = 1.852
CU4	O5		(12.55501.) 0.2960 0.2550 0.4590	D = 2.001
CU4	O8		(15.55501.) 0.2180 0.5580 0.3160	D = 2.083
CU4	O7		(14.55504.) 0.2810 0.5260 0.6890	D = 2.094
CU4	O6		(13.55501.) 0.3270 0.7550 0.4450	D = 2.390
CU4	O6		(13.54504.) 0.1730 0.2550 0.5550	D = 2.470

VECTORS FROM ATOM (5.55501.) TO ATOMS 8 THROUGH 25

MN	O16	(5.55501.) 0.5331 0.4370 0.2612	(23.55501.) 0.5730 0.1180 0.2770	D = 2.130
MN	O12		(19.55502.) 0.5980 0.5180 0.4300	D = 2.201
MN	O15		(22.55501.) 0.5000 0.7890 0.2360	D = 2.272
MN	O10		(17.55503.) 0.6080 0.5330 0.1450	D = 2.340
MN	O18		(25.55501.) 0.4840 0.1670 0.1100	D = 2.467
MN	O17		(24.55501.) 0.4710 0.1580 0.3560	D = 2.529

(((((INSTRUCTION 102)))))

0.6000000E 1 0.7000000E 1 0.8000000E 1 0.2500000E 2 0.2900000E 1 0.0000000E 0 0.0000000E 0

FROM ATOMS	TO ATOMS	WITH RADIUS OR. IF A BOX, WITH SEMIDIMENSION		
CODE (MIN MAX)	(MIN MAX)	A	B	C
102 255501. 7	8 25	2.900	0.000	0.000

[illegible]	[illegible]	([illegible])	TO ATOMS	8 THROUGH 25					
[illegible]	[illegible]	([illegible]) [illegible]			(16.55501.) 0.1810 [illegible] [illegible]			D = [illegible]	
[illegible]	[illegible]				(17.55501.) 0.1030 [illegible] 0.1450			D = [illegible]	
[illegible]	[illegible]				(18.55501.) [illegible] 0.4160 [illegible]			D = [illegible]	
[illegible]	[illegible]				(16.55501.) 0.0270 0.1040-0.0050			D = [illegible]	

ANGLES AROUND ATOM [illegible]

[illegible]	[illegible]	[illegible]	(10.55501.)	(6.55501.)	(17.55501.)	[illegible]
[illegible]	[illegible]	[illegible]	(10.55501.)	(6.55501.)	(18.55501.)	[illegible]
[illegible]	[illegible]	[illegible]	(10.55501.)	(6.55501.)	(16.55501.)	117.[illegible]
[illegible]	[illegible]	[illegible]	(17.55501.)	(6.55501.)	(18.55501.)	[illegible]
[illegible]	[illegible]	[illegible]	(17.55501.)	(6.55501.)	(16.55501.)	[illegible]
[illegible]	[illegible]	[illegible]	(18.55501.)	(6.55501.)	(16.55501.)	[illegible]

VECTORS FROM ATOM (7.55501.) TO ATOMS 8 THROUGH 25

[illegible]	[illegible]	(7.55501.) 0.2950 0.7010 0.4000	(13.55501.) 0.3270 0.7550 0.4450	D = 1.[illegible]
[illegible]	014		(21.55501.) 0.4230 0.9140 0.5200	D = 1.[illegible]
[illegible]	012		(19.55501.) 0.4020 0.5180 0.5700	D = 1.477
[illegible]	013		(20.55501.) 0.4160 0.5560 0.3720	D = 1.542

ANGLES AROUND ATOM 7

[illegible]	S2	014	(13.55501.)	(7.55501.)	(21.55501.)	103.77
[illegible]	S2	012	(13.55501.)	(7.55501.)	(19.55501.)	110.[illegible]
[illegible]	S2	013	(13.55501.)	(7.55501.)	(20.55501.)	109.45
014	S2	012	(21.55501.)	(7.55501.)	(19.55501.)	117.[illegible]
014	S2	013	(21.55501.)	(7.55501.)	(20.55501.)	116.35
012	S2	013	(19.55501.)	(7.55501.)	(20.55501.)	[illegible]

(((((INSTRUCTION 102)))))
0.2200000E 2 0.2500000E 2 0.8000000E 1 0.2500000E 2 0.3100000E 1 0.0000000E 0 0.0000000E 0

FROM ATOMS	TO ATOMS	WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSION		
CODE (MIN MAX)	(MIN MAX)	A	B	C
102 22.55501. 25	8 25	3.100	0.000	0.000

VECTORS FROM ATOM (22.55501.) TO ATOMS 8 THROUGH 25

015	016	(22.55501.) 0.5000 0.7890 0.2360	(23.56501.) 0.5730 1.1180 0.2770	D = 2.551
015	09		(16.55404.) 0.4130 0.6040 0.0650	D = 2.685
015	018		(25.56501.) 0.4840 1.1670 0.1100	D = 2.700
015	017		(24.56501.) 0.4710 1.1580 0.3560	D = 2.761
015	013		(20.55501.) 0.4160 0.5860 0.3720	D = 2.869
015	011		(18.55503.) 0.5830 0.9160 0.0690	D = 2.936
015	014		(21.55502.) 0.5770 0.9140 0.4800	D = 3.035

ANGLES AROUND ATOM 22

016	015	09	(23.56501.)	(22.55501.)	(16.55404.)	142.58
016	015	018	(23.56501.)	(22.55501.)	(25.56501.)	55.58
016	015	017	(23.56501.)	(22.55501.)	(24.56501.)	57.11
016	015	013	(23.56501.)	(22.55501.)	(20.55501.)	132.88
016	015	011	(23.56501.)	(22.55501.)	(18.55503.)	58.14
016	015	014	(23.56501.)	(22.55501.)	(21.55502.)	54.34
09	015	018	(16.55404.)	(22.55501.)	(25.56501.)	88.87
09	015	017	(16.55404.)	(22.55501.)	(24.56501.)	120.01
09	015	013	(16.55404.)	(22.55501.)	(20.55501.)	76.43
09	015	011	(16.55404.)	(22.55501.)	(18.55503.)	95.09
09	015	014	(16.55404.)	(22.55501.)	(21.55502.)	162.00
018	015	017	(25.56501.)	(22.55501.)	(24.56501.)	62.40
018	015	013	(25.56501.)	(22.55501.)	(20.55501.)	128.07
018	015	011	(25.56501.)	(22.55501.)	(18.55503.)	58.22
018	015	014	(25.56501.)	(22.55501.)	(21.55502.)	104.72
017	015	013	(24.56501.)	(22.55501.)	(20.55501.)	82.49
017	015	011	(24.56501.)	(22.55501.)	(18.55503.)	108.52
017	015	014	(24.56501.)	(22.55501.)	(21.55502.)	59.36
013	015	011	(20.55501.)	(22.55501.)	(18.55503.)	168.63

(21.55502.)
(21.55502.)

TO ATOMS 8 THROUGH 25

(25.55501.) 0.4840 0.1670 0.1100 D = 2.452
(21.54501.) 0.4710 0.1580 0.3560 D = 2.723
(22.54501.) 0.5000-0.2110 0.2360 D = 2.761
(21.54502.) 0.5770-0.0860 0.4800 D = 2.880
(18.54503.) 0.5870-0.0840 0.0690 D = 2.907
(19.55502.) 0.5980 0.5180 0.4300 D = 2.911

ANGLES AROUND ATOM 23

016	016	017	(25.55501.)	(23.55501.) (24.55501.)	68.72
016	016	018	(25.55501.)	(23.55501.) (22.54501.)	65.30
016	016	014	(25.55501.)	(23.55501.) (21.54502.)	108.93
016	016	011	(25.55501.)	(23.55501.) (18.54503.)	44.50
016	016	012	(25.55501.)	(23.55501.) (19.55502.)	113.03
017	016	018	(24.55501.)	(23.55501.) (22.54501.)	65.50
017	016	014	(24.55501.)	(23.55501.) (21.54502.)	65.23
017	016	011	(24.55501.)	(23.55501.) (18.54503.)	1.20
017	016	012	(24.55501.)	(23.55501.) (19.55502.)	78.34
018	016	014	(22.54501.)	(23.55501.) (21.54502.)	70.59
018	016	011	(22.54501.)	(23.55501.) (18.54503.)	69.11
018	016	012	(22.54501.)	(23.55501.) (19.55502.)	142.43
014	016	011	(21.54502.)	(23.55501.) (18.54503.)	123.34
014	016	012	(21.54502.)	(23.55501.) (19.55502.)	85.16
011	016	012	(18.54503.)	(23.55501.) (19.55502.)	147.48

VECTORS FROM ATOM (24.55501.) TO ATOMS 8 THROUGH 25

017	016	(24.55501.) 0.4710 0.1580 0.3560	(23.55501.) 0.5730 0.1180 0.2770	D = 2.723
017	014		(21.54501.) 0.4230-0.0840 0.5200	D = 2.723
017	015		(22.54501.) 0.5000-0.2110 0.2360	D = 2.761
017	018		(25.55501.) 0.4840 0.1670 0.1100	D = 2.832
017	014		(21.54502.) 0.5770-0.0860 0.4800	D = 2.880
017	013		(20.55501.) 0.4160 0.5860 0.3720	D = 2.898

ANGLES AROUND ATOM 24

016	017	014	(23.55501.)	(24.55501.) (21.54501.)	130.49
016	017	015	(23.55501.)	(24.55501.) (22.54501.)	57.30
016	017	018	(23.55501.)	(24.55501.) (25.55501.)	53.97
016	017	014	(23.55501.)	(24.55501.) (21.54502.)	56.55
016	017	013	(23.55501.)	(24.55501.) (20.55501.)	120.25
014	017	015	(21.54501.)	(24.55501.) (22.54501.)	91.85
014	017	018	(21.54501.)	(24.55501.) (25.55501.)	142.26
014	017	014	(21.54501.)	(24.55501.) (21.54502.)	76.13
014	017	013	(21.54501.)	(24.55501.) (20.55501.)	103.88
015	017	018	(22.54501.)	(24.55501.) (25.55501.)	57.75
015	017	014	(22.54501.)	(24.55501.) (21.54502.)	65.06
015	017	013	(22.54501.)	(24.55501.) (20.55501.)	154.55
018	017	014	(25.55501.)	(24.55501.) (21.54502.)	105.54
018	017	013	(25.55501.)	(24.55501.) (20.55501.)	99.17
014	017	013	(21.54502.)	(24.55501.) (20.55501.)	137.79

VECTORS FROM ATOM (25.55501.) TO ATOMS 8 THROUGH 25

018	016	(25.55501.) 0.4840 0.1670 0.1100	(23.55501.) 0.5730 0.1180 0.2770	D = 2.452
018	018		(25.55402.) 0.5160 0.1670-0.1100	D = 2.687
018	015		(22.54501.) 0.5000-0.2110 0.2360	D = 2.700
018	011		(18.54404.) 0.4170-0.0840-0.0690	D = 2.728
018	011		(18.54503.) 0.5830-0.0840 0.0690	D = 2.750
018	017		(24.55501.) 0.4710 0.1580 0.3560	D = 2.829
018	09		(16.55404.) 0.4130 0.6040 0.0650	D = 3.082

ANGLES AROUND ATOM 25

016	018	018	(23.55501.)	(25.55501.) (25.55402.)	113.74
016	018	015	(23.55501.)	(25.55501.) (22.54501.)	59.13
016	018	011	(23.55501.)	(25.55501.) (18.54404.)	137.20

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(((( INSTRUCTION  -1 ))))
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010	011	(23,55501.)	(23,55501.)	(18,54503.)	61.02
012	017	(23,55501.)	(25,55501.)	(24,55501.)	57.10
010	09	(23,55501.)	(25,55501.)	(16,55404.)	122.14
010	010	(25,55402.)	(25,55501.)	(22,54501.)	115.34
010	011	(25,55402.)	(25,55501.)	(18,54404.)	91.02
010	017	(25,55402.)	(25,55501.)	(18,54503.)	60.22
010	09	(25,55402.)	(25,55501.)	(24,55501.)	170.83
010	011	(25,55402.)	(25,55501.)	(16,55404.)	93.13
010	011	(22,54501.)	(25,55501.)	(18,54404.)	94.49
010	017	(22,54501.)	(25,55501.)	(18,54503.)	65.13
010	09	(22,54501.)	(25,55501.)	(24,55501.)	59.86
010	011	(18,54404.)	(25,55501.)	(18,54503.)	83.68
011	017	(18,54404.)	(25,55501.)	(24,55501.)	123.28
011	09	(18,54404.)	(25,55501.)	(16,55404.)	100.62
011	017	(18,54503.)	(25,55501.)	(24,55501.)	111.99
011	09	(18,54503.)	(25,55501.)	(16,55404.)	147.18
017	09	(24,55501.)	(25,55501.)	(16,55404.)	92.30

```
                                                    ( 19,55501.) 0.4020 0.5180 0.5700      D = 1.477
                                                    ( 20,55501.) 0.4160 0.5860 0.3720      D = 1.562
 55     613

 INPUT INSTRUCTION (OK YYYY)
 0.5000000E 1  0.2500000E  2  0.8000000E  1  0.3500000E  2  0.3200000E  1  0.0000000E  0  0.0000000E  0

     FROM ATOMS     TO ATOMS        WITH RADIUS OR, IF A BOX, WITH SEMIDIMENSION
CODE (MIN  MAX)    (MIN  MAX)                          A       B       C

101  855501.  25      8   25                          3.200    0.000   0.000


VECTORS FROM ATOM (  8,55501.)     TO ATOMS   8 THROUGH  25
   01     07     (  8,55501.) 0.3060 0.0230 0.1870    ( 14,55501 ) 0.2190 0.0260 0.3110      D = 2.546
   01     02                                          (  9,54501.) 0.2910-0.4590 0.1670      D = 2.771
   01     04                                          ( 11,54404.) 0.3050 0.2360-0.0610      D = 3.072
   01     04                                          ( 11,54501.) 0.1950-0.2640 0.0610      D = 3.106
   01     04                                          ( 10,55501.) 0.1810 0.2670 0.0740      D = 3.154
   01     03                                          (  9,55501.) 0.2910 0.5410 0.1670      D = 3.190
   01     02

VECTORS FROM ATOM (  9,55501.)     TO ATOMS   8 THROUGH  25
   02     04     (  9,55501.) 0.2910 0.5410 0.1670    ( 11,55501.) 0.1950 0.7360 0.0610      D = 2.505
   02     08                                          ( 15,55501.) 0.2180 0.5580 0.3160      D = 2.511
   02     03                                          ( 10,55501.) 0.1810 0.2670 0.0740      D = 2.749
   02     01                                          (  8,56501.) 0.3060 1.0230 0.1870      D = 2.971
   02     09                                          ( 16,55404.) 0.4130 0.6040 0.0650      D = 3.099 <
   02     01                                          (  8,55501.) 0.3060 0.0230 0.1870      D = 3.190
   02     03                                          ( 10,55404.) 0.3190 0.7670-0.0740      D = 3.196

VECTORS FROM ATOM ( 10,55501.)     TO ATOMS   8 THROUGH  25
   03     011    ( 10,55501.) 0.1810 0.2670 0.0740    ( 18,55501.) 0.0830 0.4160 0.0690      D = 2.307
   03     010                                         ( 17,55501.) 0.1080 0.0330 0.1450      D = 2.380
   03     09                                          ( 16,55501.) 0.0870 0.1040-0.0650      D = 2.536
   03     04                                          ( 11,55501.) 0.1950 0.7360 0.0610      D = 2.892
   03     02                                          (  9,55501.) 0.2910 0.5410 0.1670      D = 2.949
   03     07                                          ( 14,55501.) 0.2190 0.0260 0.3110      D = 3.022
   03     01                                          (  8,55501.) 0.3060 0.0230 0.1870      D = 3.154
   03     02                                          (  9,54404.) 0.2090 0.0410-0.1670      D = 3.196

VECTORS FROM ATOM ( 11,55501.)     TO ATOMS   8 THROUGH  25
   04     02     ( 11,55501.) 0.1950 0.7360 0.0610    (  9,55501.) 0.2910 0.5410 0.1670      D = 2.505
   04     03                                          ( 10,55501.) 0.1810 0.2670 0.0740      D = 2.892
   04     010                                         ( 17,56501.) 0.1080 1.0330 0.1450      D = 2.902
   04     08                                          ( 15,55501.) 0.2180 0.5580 0.3160      D = 3.019
   04     01                                          (  8,55404.) 0.1940 0.5230-0.1670      D = 3.072
   04     01                                          (  8,56501.) 0.3060 1.0230 0.1870      D = 3.106
   04     011                                         ( 18,55501.) 0.0830 0.4160 0.0690      D = 3.137 >

VECTORS FROM ATOM ( 12,55501.)     TO ATOMS   8 THROUGH  25
   05     07     ( 12,55501.) 0.2960 0.2550 0.4590    ( 14,55501.) 0.2190 0.0260 0.3110      D = 2.550
   05     08                                          ( 15,55501.) 0.2180 0.5580 0.3160      D = 2.808
   05     08                                          ( 15,54504.) 0.2820 0.0580 0.6840      D = 2.866
   05     012                                         ( 19,55501.) 0.4020 0.5180 0.5700      D = 2.897 >
   05     06                                          ( 13,54504.) 0.1730 0.2550 0.5550      D = 3.060
   05     07                                          ( 14,55504.) 0.2810 0.5260 0.6890      D = 3.137
   05     06                                          ( 13,55501.) 0.3270 0.7550 0.4450      D = 3.142
   05     06                                          ( 13,54501.) 0.3270-0.2450 0.4450      D = 3.142

VECTORS FROM ATOM ( 13,55501.)     TO ATOMS   8 THROUGH  25
   06     014    ( 13,55501.) 0.3270 0.7550 0.4450    ( 21,55501.) 0.4230 0.9140 0.5200      D = 2.315
   06     012                                         ( 19,55501.) 0.4020 0.5180 0.5700      D = 2.426
   06     013                                         ( 20,55501.) 0.4160 0.5860 0.3720      D = 2.462
   06     08                                          ( 15,55501.) 0.2180 0.5580 0.3160      D = 2.810
   06     07                                          ( 14,56501.) 0.2190 1.0260 0.3110      D = 3.037
   06     05                                          ( 13,55504.) 0.2040 0.7550 0.5410      D = 3.060
   06     05                                          ( 13,56501.) 0.2960 1.2550 0.4590      D = 3.142
```

(12,55501.) 0.2960 0.2550 0.4590 D = 3.142

VECTORS FROM ATOM (14,55501.) TO ATOMS 8 THROUGH 25

07	01	(14,55501.) 0.2190 0.0260 0.3110	(8,55501.)	0.3060 0.0330 0.1870	D = 2.546
07	05		(12,55501.)	0.2960 0.2550 0.4590	D = 2.550
07	010		(17,55501.)	0.1080 0.0330 0.1450	D = 2.764
07	06		(15,54501.)	0.2180-0.4420 0.3160	D = 2.864
07	03		(10,55501.)	0.1810 0.2670 0.0740	D = 3.022
07	04		(13,54501.)	0.3270-0.2450 0.4450	D = 3.037
07	05		(12,54504.)	0.2040-0.2450 0.5410	D = 3.137
07	012		(19,54504.)	0.0980 0.0180 0.4300	D = 3.161

VECTORS FROM ATOM (15,55501.) TO ATOMS 8 THROUGH 25

08	02	(15,55501.) 0.2180 0.5580 0.3160	(9,55501.)	0.2910 0.5410 0.1670	D = 2.511
08	05		(12,55501.)	0.2960 0.2550 0.4590	D = 2.809
08	06		(13,55501.)	0.3270 0.7550 0.4450	D = 2.810
08	07		(14,56501.)	0.2190 1.0260 0.3110	D = 2.864
08	05		(12,55504.)	0.2040 0.7550 0.5410	D = 2.866
08	04		(11,55501.)	0.1950 0.7360 0.0610	D = 3.019
08	016		(23,45503.)	0.0730 0.6180 0.2770	D = 3.121

VECTORS FROM ATOM (16,55501.) TO ATOMS 8 THROUGH 25

09	010	(16,55501.) 0.0870 0.1040-0.0650	(17,55501.)	0.1080 0.0330 0.1450	D = 2.359
09	011		(18,55501.)	0.0830 0.4160 0.0690	D = 2.442
09	03		(10,55501.)	0.1810 0.2670 0.0740	D = 2.536
09	015		(22,54404.)	0.0000 0.2890-0.2360	D = 2.685
09	018		(25,54404.)	0.0160-0.3330-0.1100	D = 3.082
09	02		(9,54404.)	0.2090 0.0410-0.1670	D = 3.099

VECTORS FROM ATOM (17,55501.) TO ATOMS 8 THROUGH 25

010	09	(17,55501.) 0.1080 0.0330 0.1450	(16,55501.)	0.0870 0.1040-0.0650	D = 2.359
010	03		(10,55501.)	0.1810 0.2670 0.0740	D = 2.380
010	011		(18,55501.)	0.0830 0.4160 0.0690	D = 2.519
010	07		(14,55501.)	0.2190 0.0260 0.3110	D = 2.764
010	04		(11,54501.)	0.1950-0.2640 0.0610	D = 2.902
010	016		(23,44503.)	0.0730-0.3820 0.2770	D = 3.104
010	015		(22,44503.)	0.0000 0.2890 0.2360	D = 3.144

VECTORS FROM ATOM (18,55501.) TO ATOMS 8 THROUGH 25

011	03	(18,55501.) 0.0830 0.4160 0.0690	(10,55501.)	0.1810 0.2670 0.0740	D = 2.307
011	09		(16,55501.)	0.0870 0.1040-0.0650	D = 2.442
011	010		(17,55501.)	0.1080 0.0330 0.1450	D = 2.519
011	016		(23,45503.)	0.0730 0.6180 0.2770	D = 2.687
011	018		(25,55404.)	0.0160 0.6670-0.1100	D = 2.728
011	018		(25,45503.)-0.0160 0.6670 0.1100		D = 2.750
011	015		(22,44503.)	0.0000 0.2890 0.2360	D = 2.936
011	04		(11,55501.)	0.1950 0.7360 0.0610	D = 3.137

VECTORS FROM ATOM (19,55501.) TO ATOMS 8 THROUGH 25

012	013	(19,55501.) 0.4020 0.5180 0.5700	(20,55501.)	0.4160 0.5860 0.3720	D = 2.337
012	06		(13,55501.)	0.3270 0.7550 0.4450	D = 2.426
012	014		(21,55501.)	0.4230 0.9140 0.5200	D = 2.547
012	05		(12,55501.)	0.2960 0.2550 0.4590	D = 2.897
012	016		(23,55502.)	0.4270 0.1180 0.7230	D = 2.982
012	07		(14,55504.)	0.2810 0.5260 0.6890	D = 3.161

VECTORS FROM ATOM (20,55501.) TO ATOMS 8 THROUGH 25

013	012	(20,55501.) 0.4160 0.5860 0.3720	(19,55501.)	0.4020 0.5180 0.5700	D = 2.337
013	06		(13,55501.)	0.3270 0.7550 0.4450	D = 2.462
013	014		(21,55501.)	0.4230 0.9140 0.5200	D = 2.592
013	015		(23,55501.)	0.5000 0.7890 0.2360	D = 2.869
013	017		(24,55501.)	0.4710 0.1580 0.3560	D = 2.898

VECTORS FROM ATOM (21,55501.) TO ATOMS 8 THROUGH 25

014	06	(21,55501.) 0.4230 0.9140 0.5200	(13,55501.)	0.3270 0.7550 0.4450	D = 2.315
014	012		(19,55501.)	0.4020 0.5180 0.5700	D = 2.547

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  O14     O13                                            ( 23,56502.) 0.4370 1.1180 0.7230      D = 2.597
  O14     O13                                            ( 20,55501.) 0.4160 0.5860 0.3720      D = 2.592
  O14     O17                                            ( 24,56501.) 0.4710 1.1580 0.3560      D = 2.723
  O14     O17                                            ( 24,56501.) 0.5790 1.1580 0.6440      D = 2.800
  O14     O15                                            ( 22,55502.) 0.5000 0.7890 0.7640      D = 3.033

VECTORS FROM ATOM  ( 22,55501.)      TO ATOMS    8 THROUGH  25
  O15     O16      ( 22,55501.) 0.5000 0.7890 0.2360     ( 23,56501.) 0.5730 1.1180 0.2770      D = 2.551
  O15     O9                                             ( 16,55404.) 0.4130 0.6040 0.0650      D = 2.683
  O15     O18                                            ( 25,56501.) 0.4840 1.1670 0.1100      D = 2.700
  O15     O17                                            ( 24,56501.) 0.4710 1.1580 0.3560      D = 2.761
  O15     O13                                            ( 20,55501.) 0.4160 0.5860 0.3720      D = 2.859
  O15     O11                                            ( 18,55503.) 0.5830 0.9160 0.0690      D = 2.736
  O15     O14                                            ( 21,55502.) 0.5770 0.9140 0.4800      D = 3.033
  O15     O10                                            ( 17,55503.) 0.6080 0.5330 0.1450      D = 3.144

VECTORS FROM ATOM  ( 23,55501.)      TO ATOMS    8 THROUGH  25
  O16     O18      ( 23,55501.) 0.5730 0.1180 0.2770     ( 25,55501.) 0.4840 0.1670 0.1100      D = 2.452
  O16     O17                                            ( 24,55501.) 0.4710 0.1580 0.3560      D = 2.546
  O16     O15                                            ( 22,54501.) 0.5000-0.2110 0.2360      D = 2.551
  O16     O14                                            ( 21,54502.) 0.5770-0.0860 0.4800      D = 2.597
  O16     O11                                            ( 18,54503.) 0.5830-0.0840 0.0690      D = 2.687
  O16     O12                                            ( 19,55502.) 0.5980 0.5180 0.4300      D = 2.902
  O16     O10                                            ( 17,55503.) 0.6080 0.5330 0.1450      D = 3.104
  O16     O8                                             ( 15,54503.) 0.7180 0.0580 0.3160      D = 3.121

VECTORS FROM ATOM  ( 24,55501.)      TO ATOMS    8 THROUGH  25
  O17     O16      ( 24,55501.) 0.4710 0.1580 0.3560     ( 23,55501.) 0.5730 0.1180 0.2770      D = 2.546
  O17     O14                                            ( 21,54501.) 0.4230-0.0860 0.5200      D = 2.723
  O17     O15                                            ( 22,54501.) 0.5000-0.2110 0.2360      D = 2.761
  O17     O18                                            ( 25,55501.) 0.4840 0.1670 0.1100      D = 2.829
  O17     O14                                            ( 21,54502.) 0.5770-0.0860 0.4800      D = 2.880
  O17     O13                                            ( 20,55501.) 0.4160 0.5860 0.3720      D = 2.898

VECTORS FROM ATOM  ( 25,55501.)      TO ATOMS    8 THROUGH  25
  O18     O16      ( 25,55501.) 0.4840 0.1670 0.1100     ( 23,55501.) 0.5730 0.1180 0.2770      D = 2.452
  O18     O18                                            ( 25,55402.) 0.5160 0.1670-0.1100      D = 2.687
  O18     O15                                            ( 22,54501.) 0.5000-0.2110 0.2360      D = 2.700
  O18     O11                                            ( 18,54404.) 0.4170-0.0840-0.0690      D = 2.728
  O18     O11                                            ( 18,54503.) 0.5830-0.0840 0.0690      D = 2.750
  O18     O17                                            ( 24,55501.) 0.4710 0.1580 0.3560      D = 2.829
  O18     O9                                             ( 16,55404.) 0.4130 0.6040 0.0650      D = 3.082

    ((((( INSTRUCTION    -1 )))))
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TABLE 4

Menchetti S. & Sabelli C. Campigliaite. Anisotropic thermal parameters.

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu(1)	.0006(1)	.0203(21)	.0003(4)	.0015(7)	.0004(1)	.0007(12)
Cu(2)	.0015(2)	.0077(29)	.0026(6)	-.0022(8)	.0010(3)	-.0026(17)
Cu(3)	.0005(1)	.0171(36)	.0005(5)	.0006(8)	.0002(2)	.0025(18)
Cu(4)	.0006(1)	.0193(24)	.0003(4)	.0008(8)	.0003(1)	.0001(13)
Mn	.0007(2)	.0357(14)	.0015(7)	-.0016(7)	.0006(2)	.0016(14)
S(1)	.0015(3)	.0321(85)	.0001(9)	-.0019(12)	-.0002(4)	.0015(22)
S(2)	.0014(3)	.0028(49)	.0009(10)	.0002(10)	-.0004(4)	.0000(16)
O(1)	.0018(10)	.0143(150)	.0007(31)	-.0009(21)	.0010(8)	-.0015(52)
O(2)	.0008(7)	.0164(151)	.0013(28)	.0008(26)	-.0005(11)	.0035(53)
O(3)	.0007(6)	.0497(143)	.0011(22)	-.0015(25)	.0002(10)	-.0070(48)
O(4)	.0012(8)	.0253(128)	.0018(20)	.0020(28)	-.0009(8)	-.0034(32)
O(5)	.0013(10)	.0127(112)	.0036(27)	-.0013(30)	.0004(9)	-.0045(51)
O(6)	.0016(9)	.0264(180)	.0027(30)	.0005(21)	.0013(12)	.0053(62)
O(7)	.0016(7)	.0057(98)	.0031(33)	.0005(22)	-.0001(8)	-.0041(48)
O(8)	.0008(8)	.0220(115)	.0018(29)	-.0042(27)	.0012(9)	-.0057(53)
O(9)	.0016(9)	.0592(265)	.0057(37)	-.0032(34)	.0003(15)	-.0169(68)
O(10)	.0003(6)	.0511(195)	.0104(41)	.0040(45)	.0013(13)	.0168(102)
O(11)	.0019(11)	.0029(113)	.0152(41)	-.0006(29)	.0000(17)	-.0039(63)
O(12)	.0018(12)	.1388(413)	.0005(32)	-.0026(34)	.0000(15)	-.0044(74)
O(13)	.0032(10)	.0398(198)	.0038(33)	.0079(33)	.0003(15)	-.0077(63)
O(14)	.0015(9)	.0032(121)	.0027(33)	.0002(24)	.0010(14)	-.0024(52)
O(15)	.0018(7)	.0101(96)	.0075(34)	-.0014(34)	.0014(13)	-.0086(69)
O(16)	.0029(12)	.0019(82)	.0055(38)	.0018(30)	.0013(17)	.0027(54)
O(17)	.0020(9)	.0621(209)	.0039(32)	.0083(33)	.0015(14)	.0148(65)
O(18)	.0018(10)	.0560(189)	.0130(41)	.0027(32)	.0043(18)	-.0022(59)

Form of anisotropic temperature factors: $\exp -(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)$