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AFFILIATIONS

[1]G I I ,C fG , 430074, C
[2]I fM , A f , 47, K 04001,
[3] fE M , M , fL , L E1 4N , K I
[4]N K L f D I fF , C A I fE , M 621900, C
[5]N L , H I , 11 0L , K I
[6]E L , F I , G 9 9 , K I
[7] f , L , L 730000, C

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[b)]Author to whom correspondence should be addressed: @ .

ABSTRACT

M
. H , -
. , - A
,
D . H , A B 5.25L 0.75F C 3O18
.
A , *in situ*
F 3+ O F 3+, C 3+ O C 3+, F 3+ O C 3+ - .
. A , C /F -
, - .

M (FE) A B 5F 3O15 (=4) B 6F 2 3O18 (FM) (=5), B 4 3O12
, , BF O3, FE FM .[12,13] B -
, .[1 4] H , - C F B- , B 5F 0.5C 0.5 3O15
- (=4) B 6F C 3O18 (=5)
.[5] , - A
(B 2O2)2+(A -1B O 3 +1)2− (A -, .[14,15] H ,
-, 12- - , B
- ,
D -
)[6] .[16] , -
B- - A
BF O3 - .[7 11] .

I , A B 5.25L 0.75F C 3O18 (BLFC) ( ). L

C , F , .[14,17] D A

a b , BLFC a b . A

- , .[18] -

A , *in situ* I H I I N , AL, D , O , K. F

( ). , A BLFC

. BLFC . , - ,

F 1 - (D) BLFC . A *B2cb* - A ,

A2$_1$, A .[19,20] *B2cb* a = 5.4530(2) A, b = 5.4427(1) A, c = 50.670(2) A - *A2*$_1$*am* a = 5.4651(6) A, b = 5.3943(6) A, c = 41.487(2) A F (:// . .).

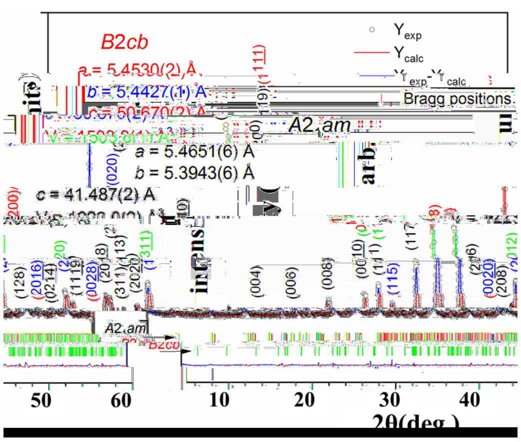

FIG. 1. -

BLFC - A =4 =5 . N D'

. F 1 EM BLFC . - (a–b) . M ,

F . 1 . - 1.4 . %, D. ED (F . 2 1)

F , C , O, . , C 2F O4 -

. - A B 5F 0.5C 0.5 3O15.[16] F 2( )

BLFC (50, 70 100, 300, 500 H). 1060 K FE T BLFC . H , BLFC B 6 3F 2O18 (973 K).[13] F 2( ) *P–E* *I–E* BLFC . *I–E* ,[21,22] . BLFC 10 μC/ 2.

F 2( ) - (FC) - (FC) 200 O BLFC . BLFC

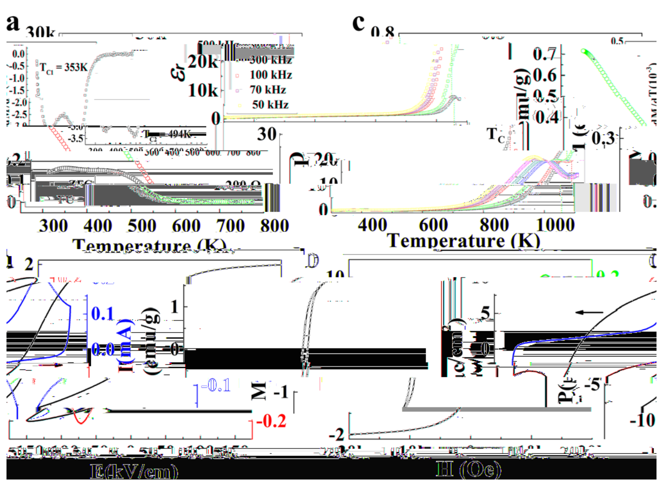

FIG. 2. ( ) = 200 300

$_1 \sim 494$ K
(M/),
$B_6F\ C\ _3O_{18}$ (526 K).[23]
BLFC
F^{3+} O F^{3+}, C^{3+} O C^{3+}, F^{3+} O C^{3+} (.
).[24]
ED .
A FC $_2 \sim 353$ K
$C_2F\ O_4$. $_2$
$C_2F\ O_4$ (460 K) .[16,25]
(M) $C_2F\ O_4$
16 23.5 / .[25] , 1.4 .%
C_2 F O_4 0.22 0.32 / ,
BLFC
M = 1.85 / , F . 2( ). I
, M H
$_1$
$_2$ (F . 3).
425 K 1.58 / .
0.27 / ,
ED
. , BLFC
A .
F 3
F^{3+} O C^{3+}
(DF) *ab initio*
(A) . H
$_F = 2$ $_C = 3$ F C , ,
(GGA)+ . I
BLFC
F . 3( ), F^{3+} C^{3+} (3.1 2.1 μ_B/ ,),
O
(0.1 μ_B/).
F O_6 C O_6
( ) F /C
F O - / . F . 3( ).
F ,
F^{3+} C^{3+} ,
(. .,) (. .,
) , .
, $E_{FM} - E_{AFM}$
= −144.1 .
H , . (FM)
43.5 (. ., 504.6 K), FM
$_1$ FC/FC . F . 2( ).
a b
. ,
010 .
F 4
BLFC . I
- , - ,

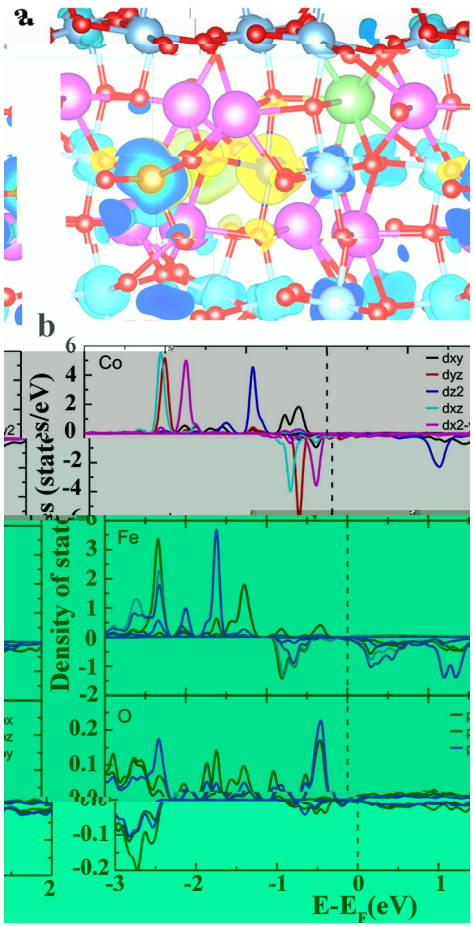

FIG. 3. ( ) t t tm (= 0.005) ( ), {), ( ), t), ( ), ( ) tm . ( ) t t t t t t t t $^{3+}$ $^{3+}$.

. N
,
,
. I F . 4,
A (0 1 20)
. ,
2 . F
(2 < H < 5),
2 , M H F . 2( ) 3. F ,
.
F 5
BLFC F M
399 O .
FM BLFC , F .
5( ). A F -

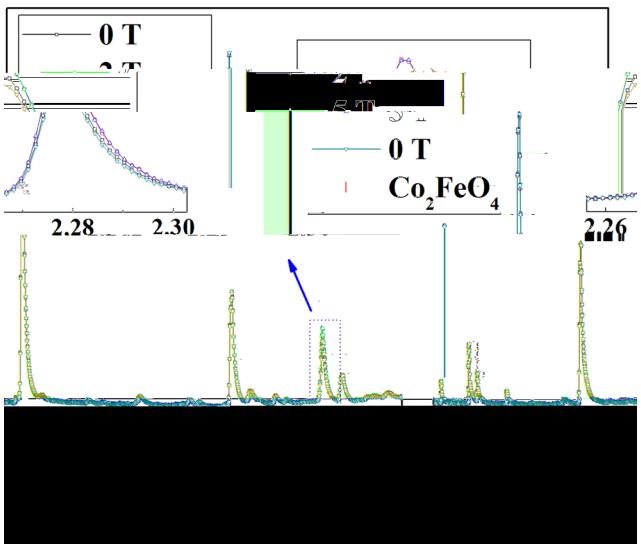

FIG. 4. , t t t t tt t t (0, 2, 5 t t, 0).

C - ( ) - +2000 O F . 5( ). −2000 O - , F . 5( ). (-) C 2F O4 - - - . , - , - A BLFC . G (*P*) 100 (*M*) 010 , (-

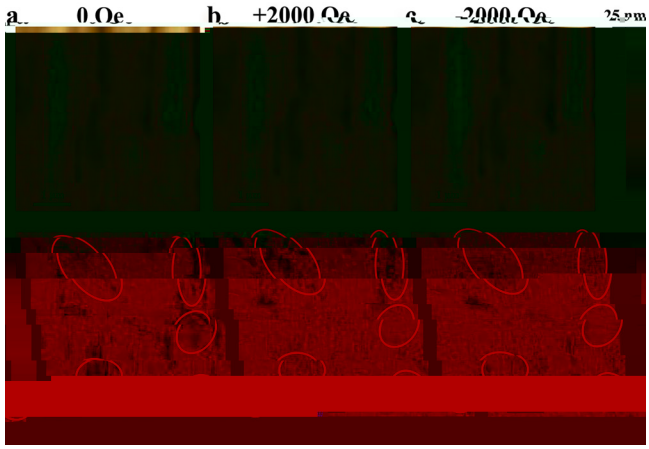

FIG. 5. t t t t (t, t t). ( ) ( ) t t 0, ( )t, ( ) t t +2000, ( ) t, ( ) t t −2000, .

) $T = P \times M$ BLFC . I , A BLFC - . F F 3+ O F 3+, C 3+ O C 3+, F 3+ O C 3+ - . - . A , C /F , - - .

, EM - (ED) , BLFC .

D . M , D . K , D. D I H I I N , AL, D , O , K. A E D F , G A A (G N . 2/0038/20), C (G N . K2015-0602006), N FC (G N . 11474138 11834005). A E M (EM) IND54 N . EM EM E AME E .

DATA AVAILABILITY

.

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