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## AFFILIATIONS

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

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## ABSTRACT

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

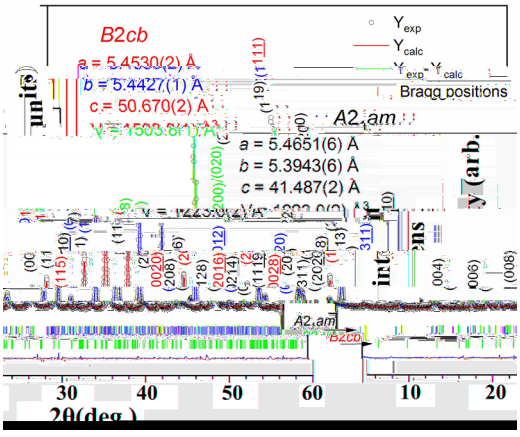


FIG. 1. - a a a B .

‾ 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 $_2$F O$_4$ - . - A B $_5$F $_{0.5}$C $_{0.5}$ ‾ $_3$O$_{15}$.[16] F 2( ) BLFC‾ (50, 70 100, 300, 500 H ).‾ 1060 K FE *T* BLFC‾. H , BLFC‾ B $_6$‾ $_3$F $_2$O$_{18}$ ( 973 K).[13] F 2( ) *P*–*E* *I*–*E* BLFC‾ ▲‾.‾ *I*–*E* ,[21,22] .‾ BLFC‾ 10 $\mu$C/ $^2$. F 2( ) - ( FC) - (FC) 200 O BLFC‾. BLFC‾

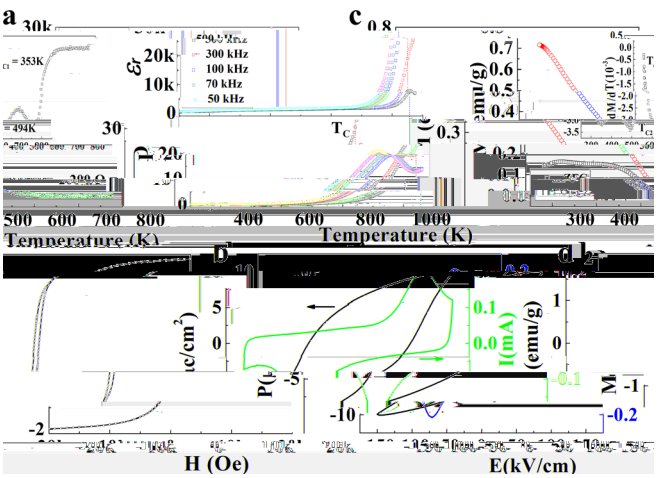


FIG. 2. (a) a a (a ) a a ( ) B a a a ⊥ . ( ) a B a a a a . ( ) a a a B a ⊥ / a = 200 . a a - a / a a a . ( ) a a- a 300 B a .

$_1 \sim 494$ K
( M/ ),
B $_6$F C $_3$O$_{18}$ (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 $_2$F O$_4$. $_2$
C $_2$F O$_4$ (460 K) .[16,25]
(M ) C $_2$F 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 $\mu_B$/ , ),
O
( 0.1 $\mu_B$/ ).
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
- , - ,

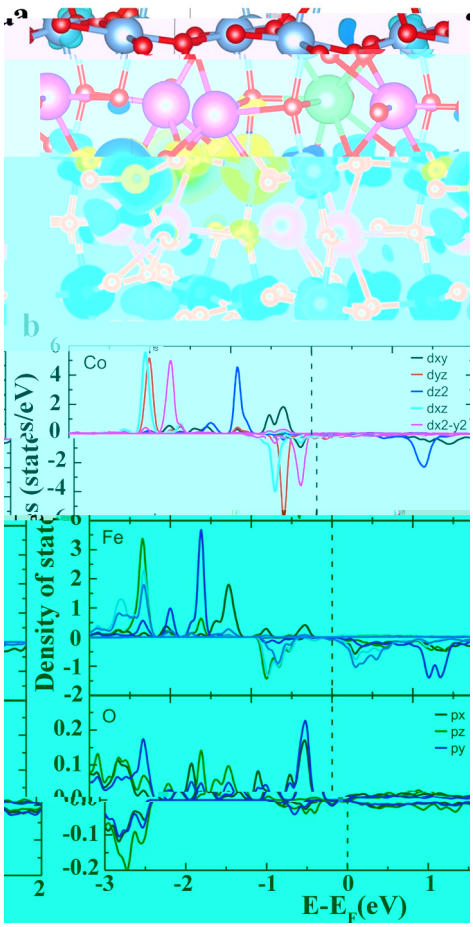


**FIG. 3.** (a) ( a = 0.005) ( ), B ( ),
a ( ), ( ), ( a ), a ( ) a . ( ) A a
a $^{3+}$ $^{3+}$.

.
. 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 -

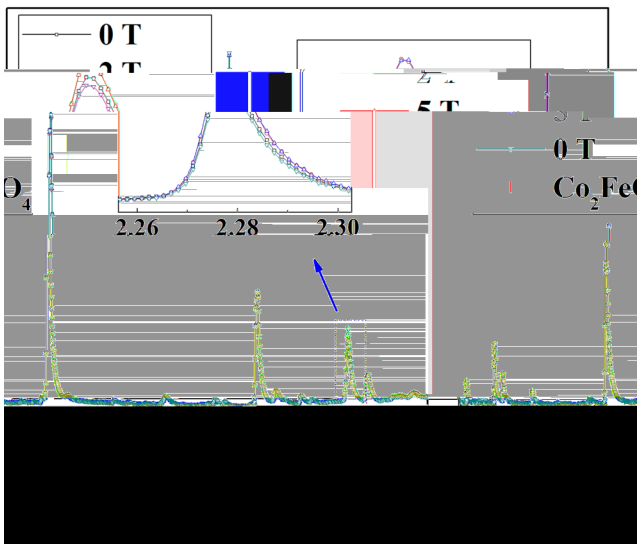


FIG. 4. - a a a a a B a a a ( 0, 2, a 5 a a 0 ).

C - ( ) - +2000 O F . 5( ). −2000 O - , F . 5( ). ( - ) C $_2$F O$_4$ - - - . , - , - A BLFC . G ($P$) 100 ($M$) 010 , ( -

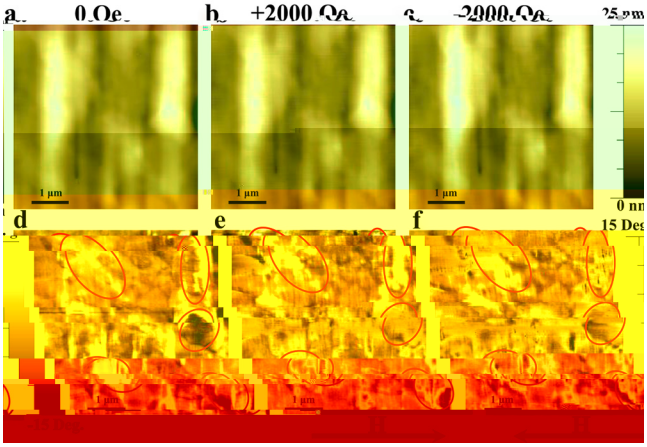


FIG. 5. a B a a ( aa a a a ). (a) a a ( ) a a a 0 ( ) a a ( ) a a a +2000 a ( ) a a ( ) a a a −2000 .

) $T = P \times M$ 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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