SUPPLEMENTARY MATERIALS

Structure Refinement of the Layered Composite Crystal $Sc_2B_{1.1}C_{3.2}$ in a Five-Dimensional Formalism

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Table I. Symmetry operations and requirement on the atomic modulation waves.
(a) Generator set of symmetry operations

Space group	Superspace group	
Subsystem 1	Subsystem 2	
(Sc_2C part)	($B_{1/3}C_{2/3}$ part)	$[Sc_2C][2(B_{1/3}C_{2/3})]_{81/49}$
a_1=3.387,	a_2=2.634,	a=3.387,
c=6.703Å	c=6.703Å	c=6.703Å,
		σ_1=(9/7 0 0), σ_2=(0 9/7 0)
x, y, z	x, y, z	x, y, z, u, v
-y, x-y, z	-y, x-y, z	-y, x-y, z, -v, u-v
-y, -x, z	-y, -x, z	-y, -x, z, -v, -u
-x, -y, -z	-x, -y, -z	-x, -y, -z, -u, -v
$P\bar{3}m1$	$P\bar{3}m1$	$P\bar{3}m1(p\ 0\ 0)(0\ p\ 0)0m0$

(b) Requirement on the atomic modulation waves. For the first subsystem $A_{i,m,n}$ and $B_{i,m,n}$ for i=x, y, z, β_{ij} are the cosine and sine amplitudes of the Fourier series with the wave vector $m\boldsymbol{a}_2^*+n\boldsymbol{b}_2^*$, and for the second subsystem $A_{i,h,k}$ and $B_{i,h,k}$ are with the wave vector $h\boldsymbol{a}_1^*+k\boldsymbol{b}_1^*$.

Subsystem 1

Sc (1/3, 2/3, z)

$A_{x,n,-m-n}=-A_{y,-m-n,m}=-A_{y,m+n,-n}=A_{x,-m,m+n}=-A_{x,m,n}+A_{y,m,n}$, $A_{y,n,-m-n}=A_{y,-n,-m}=-A_{x,m+n,-n}=-A_{x,m,n}$,

$A_{x,-m-n,m}= A_{x,-n,-m}=-A_{y,-m,m+n} =-A_{y,m,n}$, $A_{z,m,n}=A_{z,n,-m-n}=A_{z,-m-n,m}=A_{z,-n,-m} =A_{z,-m,m+n}=A_{z,m+n,-n}$,

$B_{x,n,-m-n}=-B_{y,-m-n,m}=-B_{y,m+n,-n}=B_{x,-m,m+n}=-B_{x,m,n}+B_{y,m,n}$, $B_{y,n,-m-n}=B_{y,-n,-m}=-B_{x,m+n,-n}=-B_{x,m,n}$,

$B_{x,-m-n,m}= B_{x,-n,-m}=-B_{y,-m,m+n}=-B_{y,m,n}$, $B_{z,m,n}=B_{z,n,-m-n}=B_{z,-m-n,m}=B_{z,-n,-m}=B_{z,-m,m+n}=B_{z,m+n,-n}$,

$A_{x,m,0}=2A_{y,m,0}$, $B_{x,m,0}=2B_{y,m,0}$, $A_{x,m,m}=-A_{y,m,m}$, $B_{x,m,m}=B_{y,m,m}$, $B_{z,m,m}=0$,

$A_{\beta 11,n,-m-n}=A_{\beta 22,-m-n,m}=A_{\beta 22,m+n,-n}=A_{\beta 11,-m,m+n}=A_{\beta 11,m,n}-2A_{\beta 12,m,n}+A_{\beta 22,m,n}$, $A_{\beta 22,n,-m-n}=A_{\beta 22,-n,-m}=A_{\beta 11,m+n,-n}=A_{\beta 11,m,n}$, $A_{\beta 11,-m-n,m}=A_{\beta 11,-n,-m}=A_{\beta 22,-m,m+n}=A_{\beta 22,m,n}$, $A_{\beta 12,n,-m-n}=A_{\beta 12,m+n,-n}=A_{\beta 11,m,n}-A_{\beta 12,m,n}$, $A_{\beta 12,-m-n,m}=A_{\beta 12,-m,m+n}=A_{\beta 22,m,n}-A_{\beta 12,m,n}$, $A_{\beta 12,-n,-m}=A_{\beta 12,m,n}$, $A_{\beta 13,n,-m-n}=-A_{\beta 23,-m-n,n}=-A_{\beta 23,m+n,-n}=A_{\beta 13,-m,m+n}=-A_{\beta 13,m,n}+A_{\beta 23,m,n}$, $A_{\beta 23,n,-m-n}=A_{\beta 23,-n,-m}=-A_{\beta 13,m+n,-n}=-A_{\beta 13,m,n}$, $A_{\beta 13,-m-n,m}=A_{\beta 13,-n,-m}=-A_{\beta 23,-m,m+n}=-A_{\beta 23,m,n}$, $A_{\beta 33,m,n}=A_{\beta 33,n,-m-n} =A_{\beta 33,-m-n,m}=A_{\beta 33,-n,-m} =A_{\beta 33,-m,m+n}=A_{\beta 33,m+n,-n}$,

$B_{\beta 11,n,-m-n}=B_{\beta 22,-m-n,m}=B_{\beta 22,m+n,-n}=B_{\beta 11,-m,m+n}=B_{\beta 11,m,n}-2B_{\beta 12,m,n}+B_{\beta 22,m,n}$, $B_{\beta 22,n,-m-n}=B_{\beta 22,-n,-m}=B_{\beta 11,m+n,-n}=B_{\beta 11,m,n}$, $B_{\beta 11,-m-n,m}=B_{\beta 11,-n,-m}=B_{\beta 22,-m,m+n}=B_{\beta 22,m,n}$, $B_{\beta 12,n,-m-n}=B_{\beta 12,m+n,-n}=B_{\beta 11,m,n}-B_{\beta 12,m,n}$, $B_{\beta 12,-m-n,m}=B_{\beta 12,-m,m+n}=B_{\beta 22,m,n}-B_{\beta 12,m,n}$, $B_{\beta 12,-n,-m}=B_{\beta 12,m,n}$, $B_{\beta 13,n,-m-n}=-B_{\beta 23,-m-n,n}=-B_{\beta 23,m+n,-n}=B_{\beta 13,-m,m+n}=-B_{\beta 13,m,n}+B_{\beta 23,m,n}$, $B_{\beta 23,n,-m-n}=B_{\beta 23,-n,-m}=-B_{\beta 13,m+n,-n}=-B_{\beta 13,m,n}$, $B_{\beta 13,-m-n,m}=B_{\beta 13,-n,-m}=-B_{\beta 23,-m,m+n}=-B_{\beta 23,m,n}$, $B_{\beta 33,m,n}=B_{\beta 33,n,-m-n}=B_{\beta 33,-m-n,m}=B_{\beta 33,-n,-m}=B_{\beta 33,-m,m+n}=B_{\beta 33,m+n,-n}$,

$A_{\beta 11,m,0}=2A_{\beta 12,m,0}$, $B_{\beta 11,m,0}=2B_{\beta 12,m,0}$, $A_{\beta 13,m,0}=2A_{\beta 23,m,0}$, $B_{\beta 13,m,0}=2B_{\beta 23,m,0}$

C (0, 0, 1/2)

$A_{x,m,n}=A_{x,n,-m-n}=A_{x,-m-n,m}=A_{x,-n,-m}=A_{x,m+n,-n}=A_{x,-m,m+n}=A_{y,m,n}=A_{y,n,-(m+n)}=A_{y,-(m+n),m}=A_{y,-n,-m}=A_{y,m+n,-n}=A_{y,-m,m+n}=A_{z,m,n}=A_{z,n,-m-n} =A_{z,-m-n,m}=A_{z,-n,-m}=A_{z,m+n,-n}=A_{z,-m,m+n}=0$,

$B_{x,n,-m-n}=-B_{y,-m-n,m}=-B_{y,m+n,-n}=B_{x,-m,m+n}=-B_{x,m,n}+B_{y,m,n}$, $B_{y,n,-m-n}=B_{y,-n,-m}= -B_{x,m+n,-n}=-B_{x,m,n}$,

$B_{x,-m-n,m}=B_{x,-n,-m}=-B_{y,-m,m+n}=-B_{y,m,n}$, $B_{z,m,n}=B_{z,n,-m-n}=B_{z,-m-n,m} =B_{z,-n,-m}=B_{z,m+n,-n}=B_{z,-m,m+n}$, $B_{x,m,0}=2B_{y,m,0}$

Subsystem 2

$B_{1/3}C_{2/3}$ (1/3, 2/3, z)

$A_{x,k,-h-k}=-A_{y,-h-k,h}=-A_{y,h+k,-k}=A_{x,-h,h+k}=-A_{x,h,k}+A_{y,h,k}$, $A_{y,k,-h-k}=A_{y,-k,-h}=-A_{x,h+k,-k}=-A_{x,h,k}$,

$A_{x,-h-k,h}= A_{x,-k,-h}=-A_{y,-h,h+k}=-A_{y,h,k}$, $A_{z,h,k}=A_{z,k,-h-k}=A_{z,-h-k,h}=A_{z,-k,-h} =A_{z,-h,h+k}=A_{z,h+k,-k}$,

$B_{x,k,-h-k}=-B_{y,-h-k,h}=-B_{y,h+k,-k}=B_{x,-h,h+k}=-B_{x,h,k}+B_{y,h,k}$, $B_{y,k,-h-k}=B_{y,-k,-h}=-B_{x,h+k,-k}=-B_{x,h,k}$,

$B_{x,-h-k,h}= B_{x,-k,-h}=-B_{y,-h,h+k}=-B_{y,h,k}$, $B_{z,h,k}=B_{z,k,-h-k}=B_{z,-h-k,h}=B_{z,-k,-h}=B_{z,-h,h+k}=B_{z,h+k,-k}$. $A_{x,h,0}=2A_{y,h,0}$, $B_{x,h,0}=2B_{y,h,0}$

Table II. Interatomic distances (Å) calculated from the parameters listed in Table 4 (the first model) of the text.

1)CSc$_6$ octahedral unit

		*
C$^{(155)}$		1b
-Sc$^{(155)}$,Sc$^{(7'55)}$,Sc$^{(154)}$,Sc$^{(7'56)}$,Sc$^{(144)}$,Sc$^{(7'66)}$	2.300(5)×6	
C$^{(156)}$		6h
-Sc$^{(156)}$,Sc$^{(7'57)}$,Sc$^{(155)}$,Sc$^{(7'56)}$,Sc$^{(145)}$,Sc$^{(7'67)}$	2.318(4) ×2, 2.278(4) ×2, 2.290(3) ×2	
C$^{(157)}$		6h
-Sc$^{(157)}$,Sc$^{(7'58)}$,Sc$^{(156)}$,Sc$^{(7'57)}$,Sc$^{(146)}$,Sc$^{(7'68)}$	2.289(3) ×2, 2.302(3) ×2, 2.253(2) ×2	
C$^{(158)}$		6h
-Sc$^{(158)}$,Sc$^{(7'59)}$,Sc$^{(157)}$,Sc$^{(7'58)}$,Sc$^{(147)}$,Sc$^{(7'69)}$	2.286(4) ×2, 2.299(4) ×2, 2.288(3) ×2	
C$^{(164)}$		6i
-Sc$^{(164)}$,Sc$^{(153)}$,Sc$^{(7'64)}$,Sc$^{(7'75)}$, Sc$^{(163)}$,Sc$^{(7'65)}$	2.338(4) ×2, 2.298(4) ×2, 2.347(4), 2.280(6)	
C$^{(173)}$		6i
-Sc$^{(173)}$,Sc$^{(162)}$,Sc$^{(7'73)}$,Sc$^{(7'84)}$,Sc$^{(172)}$,Sc$^{(7'74)}$	2.337(4) ×2, 2.296(3) ×2, 2.283(3), 2.223(5)	
C$^{(128)}$		6i
-Sc$^{(128)}$,Sc$^{(117)}$,Sc$^{(7'28)}$,Sc$^{(7'39)}$,Sc$^{(127)}$,Sc$^{(7'29)}$	2.282(3) ×2, 2.305(4) ×2, 2.271(6), 2.329(5)	
C$^{(168)}$		12j
-Sc$^{(168)}$,Sc$^{(7'68)}$,Sc$^{(157)}$,Sc$^{(7'69)}$,Sc$^{(167)}$,Sc$^{(7'79)}$	2.317(4), 2.259(3), 2.328(4), 2.297(4),2.281(4),2.326(4)	

1)Sc-C(<2.4 Å), M(<2.6 Å)   M= B$_{1/3}$C$_{2/3}$

		*
Sc$^{(172)}$		2d
-C$^{(172)}$,C$^{(173)}$,C$^{(183)}$	2.283(3)×3	
-M$^{[171]}$,M$^{[181]}$,M$^{[182]}$,M$^{[782]}$,M$^{[783]}$,M$^{[793]}$	2.456(5)×3, 2.523(5)×3	
Sc$^{(154)}$		6i
-C$^{(154)}$,C$^{(165)}$,C$^{(155)}$	2.278(4) ×2, 2.300(5)	
-M$^{[154]}$,M$^{[765]}$	2.345(6), 2.516(5)	
Sc$^{(145)}$		6i
-C$^{(145)}$,C$^{(156)}$,C$^{(146)}$	2.290(3) ×2, 2.280(6)	
-M$^{[145]}$,M$^{[746]}$,M$^{[757]}$	2.452(5), 2.544(4) ×2	
Sc$^{(163)}$		6i
-C$^{(163)}$,C$^{(174)}$,C$^{(164)}$	2.281(4) ×2, 2.347(4)	
-M$^{[774]}$	2.486(6)	
Sc$^{(136)}$		6i
-C$^{(136)}$,C$^{(147)}$,C$^{(137)}$	2.326(4) ×2, 2.223(5)	
-M$^{[126]}$,M$^{[137]}$,M$^{[738]}$	2.510(4) ×2, 2.543(5)	
Sc$^{(127)}$		6i
-C$^{(127)}$,C$^{(138)}$,C$^{(128)}$	2.296(3) ×2, 2.271(6)	
-M$^{[118]}$,M$^{[729]}$	2.441(5), 2.517(6)	
Sc$^{(158)}$		6i
-C$^{(169)}$,C$^{(158)}$,C$^{(159)}$	2.329(5), 2.286(4) ×2	
-M$^{[159]}$,M$^{[7610]}$,M$^{[7611]}$	2.308(6), 2.563(4) ×2	
Sc$^{(156)}$		12j
-C$^{(156)}$,C$^{(157)}$,C$^{(167)}$	2.318(4), 2.302(3), 2.338(4)	
-M$^{[156]}$,M$^{[768]}$	2.444(3), 2.503(4)	
Sc$^{(157)}$		12j
-C$^{(157)}$,C$^{(158)}$,C$^{(168)}$	2.289(3), 2.299(4), 2.328(4)	
-M$^{[158]}$,M$^{[769]}$	2.344(3), 2.499(4)	
Sc$^{(146)}$		12j
-C$^{(146)}$,C$^{(147)}$,C$^{(157)}$	2.298(4), 2.259(3), 2.253(2)	
-M$^{[146]}$,M$^{[136]}$,M$^{[147]}$,M$^{[758]}$,M$^{[748]}$,M$^{[747]}$	2.540(4),2.524(4),2.482(3),2.575(3),2.547(4),2.597(4)	
Sc$^{(173)}$		12j
-C$^{(173)}$,C$^{(174)}$,C$^{(184)}$	2.337(4), 2.317(4), 2.305(4)	
-M$^{[183]}$,M$^{[784]}$,M$^{[794]}$	2.384(3), 2.512(4), 2.507(3)	
Sc$^{(125)}$		12j
-C$^{(125)}$,C$^{(126)}$,C$^{(136)}$	2.288(3), 2.282(3), 2.297(4)	
-M$^{[115]}$,M$^{[726]}$,M$^{[727]}$	2.373(5), 2.564(4), 2.526(3)	

3)M-M (<1.6Å) M= $B_{1/3}C_{2/3}$

		*
$M^{[154]}$ - $M^{[755]}$, $M^{[766]}$, $M^{[765]}$	1.517(3) ×2, 1.507(3)	6i
$M^{[145]}$ - $M^{[746]}$, $M^{[757]}$, $M^{[756]}$	1.5182(6) ×2, 1.507(3)	6i
$M^{[163]}$ - $M^{[764]}$, $M^{[775]}$, $M^{[774]}$	1.536(4) ×2, 1.536(2)	6i
$M^{[136]}$ - $M^{[737]}$, $M^{[748]}$, $M^{[747]}$	1.548(3) ×2, 1.536(2)	6i
$M^{[172]}$ - $M^{[773]}$, $M^{[784]}$, $M^{[783]}$	1.547(4) ×2, 1.557(6)	6i
$M^{[127]}$ - $M^{[728]}$, $M^{[739]}$, $M^{[738]}$	1.534(1) ×2, 1.557(6)	6i
$M^{[181]}$ - $M^{[782]}$, $M^{[793]}$, $M^{[792]}$	1.534(1) ×2, 1.546(4)	6i
$M^{[118]}$ - $M^{[719]}$, $M^{[7210]}$, $M^{[729]}$	1.535(4) ×2, 1.546(4)	6i
$M^{[159]}$ - $M^{[7610]}$, $M^{[7611]}$, $M^{[7510]}$	1.508(3) ×2, 1.511(3)	6i
$M^{[156]}$ - $M^{[757]}$, $M^{[767]}$, $M^{[768]}$	1.554(6), 1.5182(6), 1.546(4)	12j
$M^{[175]}$ - $M^{[776]}$, $M^{[786]}$, $M^{[787]}$	1.546(4), 1.547(4), 1.536(4)	12j
$M^{[157]}$ - $M^{[758]}$, $M^{[768]}$, $M^{[769]}$	1.567(7), 1.547(4), 1.531(2)	12j
$M^{[185]}$ - $M^{[786]}$, $M^{[796]}$, $M^{[797]}$	1.531(2), 1.525(4), 1.529(2)	12j
$M^{[151]}$ - $M^{[752]}$, $M^{[762]}$, $M^{[763]}$	1.533(4), 1.518(2), 1.525(4)	12j
$M^{[168]}$ - $M^{[769]}$, $M^{[779]}$, $M^{[7710]}$	1.529(2), 1.548(3), 1.550(6)	12j
$M^{[115]}$ - $M^{[716]}$, $M^{[726]}$, $M^{[727]}$	1.508(2), 1.518(2), 1.510(2)	12j
$M^{[137]}$ - $M^{[738]}$, $M^{[748]}$, $M^{[749]}$	1.547(4), 1.550(6), 1.527(3)	12j
$M^{[183]}$ - $M^{[784]}$, $M^{[794]}$, $M^{[795]}$	1.527(3), 1.535(4), 1.510(2)	12j

Symmetry codes in the first subsystem: (1pq)x+p-5,y+q-5,z (7’pq)-x+p-5,-y+q-5,1-z
Symmetry codes in the second subsystem: [1pq]x+p-5,y+q-5,z [7pq]-x+p-5,-y+q-5,-z

* Wyckoff notation in a large superlattice unit cell, A=23.710(9) and c=6.703(2)Å, with space group P$\bar{3}$m1.

Table III. Fractional coordinates of the three-dimensional superstructure, with $P\bar{3}m1$ and a unit cell of A=23.710(9) and c=6.703(2)Å, corresponding to the first model of $Sc_2B_{1.1}C_{3.2}$. Standard deviations, estimated from errors of interatomic distances using a program BONDL, are listed in parentheses. (M= $B_{1/3}C_{2/3}$)

Atom	X	Y	z	site	*
Sc1	0.33333	-0.33333	0.3619(7)	2d	(1)
Sc2	0.0483(1)	-0.0483	0.3262(6)	6i	(10)
Sc3	-0.0993(1)	0.0993	0.3456(6)	6i	(7)
Sc4	0.1933(1)	-0.1933	0.2780(4)	6i	(12)
Sc5	-0.2360(1)	0.2360	0.3317(5)	6i	(9)
Sc6	-0.3828(1)	0.3828	0.2917(6)	6i	(11)
Sc7	0.4760(1)	-0.4760	0.3275(5)	6i	(8)
Sc8	0.0398(1)	0.2348(1)	0.2973(3)	12j	(3)
Sc9	0.0427(1)	0.3777(1)	0.3091(3)	12j	(4)
Sc10	-0.0994(1)	0.2345(1)	0.3581(2)	12j	(2)
Sc11	0.3346(1)	-0.1961(1)	0.3244(4)	12j	(5)
Sc12	-0.3761(1)	0.0969(1)	0.3317(4)	12j	(6)
C1	0.0000	0.0000	0.5000	1b	(13)
C2	0.0000	0.1436(2)	0.5000	6h	(17)
C3	0.0000	0.2854(1)	0.5000	6h	(20)
C4	0.0000	0.4280(1)	0.5000	6h	(14)
C5	0.14300(3)	-0.14300	0.4445(9)	6i	(15)
C6	0.28581(2)	-0.28581	0.4445(6)	6i	(19)
C7	-0.4281(1)	0.4281	0.4863(2)	6i	(16)
C8	0.1433(1)	0.4283(1)	0.4692(5)	12j	(18)
M1	0.0366(1)	-0.0366	-0.0162(6)	6i	(34)
M2	-0.0732(1)	0.0732	0.0166(4)	6i	(33)
M3	0.14804(3)	-0.14804	-0.0760(7)	6i	(25)
M4	-0.18537(4)	0.18537	0.0897(7)	6i	(21)
M5	0.2590(1)	-0.2590	0.0205(4)	6i	(36)
M86	-0.2963(1)	0.2963	-0.0616(6)	6i	(30)
M97	0.3708(1)	-0.3708	0.0766(6)	6i	(22)
M68	-0.4080(1)	0.4080	-0.0383(4)	6i	(27)
M79	0.48177(3)	-0.48177	-0.0149(7)	6i	(38)
M10	0.0371(1)	0.18424(1)	-0.0228(3)	12j	(26)
M11	0.25850(5)	0.0734(1)	0.0607(6)	12j	(24)
M12	0.0373(1)	0.29680(5)	-0.0252(4)	12j	(31)
M13	0.3711(1)	0.0733(1)	0.0433(4)	12j	(29)
M14	0.03681(5)	-0.3716(1)	-0.0193(4)	12j	(23)
M15	0.1477(1)	0.4076(1)	-0.0550(5)	12j	(28)
M16	-0.4087(1)	0.07315(5)	-0.0069(5)	12j	(37)
M17	-0.1846(1)	0.2974(1)	0.0162(3)	12j	(35)
M18	0.3714(1)	-0.1467(1)	0.0054(3)	12j	(32)

* Each number in a parenthesis is the atom number in TABLE 2 of Shi *et al*, *J. Solid State Chemistry*, **148**, 442-449 (1999)

Table IV. Atomic parameters of the second model. The independent standard deviations are in parentheses. $A_{m,n}$ and $B_{m,n}$ are the cosine and sine terms of the Fourier amplitudes with the wave vector $m\boldsymbol{a}_2^*+n\boldsymbol{b}_2^*$ for the first subsystem, and $A_{h,k}$ and $B_{h,k}$ are those with the wave vector $h\boldsymbol{a}_1^*+k\boldsymbol{b}_1^*$ for the second subsystem.

Subsystem 1				
Sc	x	y	z	100×U_{eq}(Å^2)
Average	0.333333	0.666667	0.32223(6)	0.773(8)
$A_{1,0}$	0.0059(1)	0.00297	0.01462(5)	-0.084(9)
$B_{1,0}$	-0.0298(1)	-0.01492	0.01118(6)	0.00(1)
$A_{0,-1}$	-0.00297	-0.00594	0.01462	-0.084
$B_{0,-1}$	0.01492	0.02984	0.01118	0.00
$A_{-1,1}$	-0.00297	0.00297	0.01462	-0.084
$B_{-1,1}$	0.01492	-0.01492	0.01118	0.00
$A_{1,1}$	-0.0007(1)	0.0007	0.00102(9)	
$B_{1,1}$	0.0042(2)	0.0042	0.0000	
$A_{1,-2}$	0.0014	0.0007	0.00102	
$B_{1,-2}$	0.0000	-0.0042	0.0000	
$A_{-2,1}$	-0.0007	-0.0014	0.00102	
$B_{-2,1}$	-0.0042	0.0000	0.0000	
$A_{2,0}$	-0.0031(2)	-0.0016	0.00027(9)	
$B_{2,0}$	0.0024(2)	0.0012	0.0008(1)	
$A_{0,-2}$	0.0016	0.0031	0.00027	
$B_{0,-2}$	-0.0012	-0.0024	0.0008	
$A_{-2,2}$	0.0016	-0.0016	0.00027	
$B_{-2,2}$	-0.0012	0.0012	0.0008	
$A_{2,1}$	0.0005(3)	0.0028(4)	-0.00030(8)	
$B_{2,1}$	-0.0008(2)	-0.0022(4)	-0.0002(1)	
$A_{1,-3}$	0.0023	-0.0005	-0.00030	
$B_{1,-3}$	-0.0013	0.0008	-0.0002	
$A_{-3,2}$	-0.0028	-0.0023	-0.00030	
$B_{-3,2}$	0.0022	0.0013	-0.0002	
$A_{-1,-2}$	-0.0028	-0.0005	-0.00030	
$B_{-1,-2}$	0.0022	0.0008	-0.0002	
$A_{-2,3}$	0.0023	0.0028	-0.00030	
$B_{-2,3}$	-0.0013	-0.0022	-0.0002	
$A_{3,-1}$	0.0005	-0.0023	-0.00030	
$B_{3.-1}$	-0.0008	0.0013	-0.0002	
$A_{3,0}$	0.0049(3)	0.0024	-0.0017(2)	
$B_{3,0}$	-0.0009(4)	-0.0005	-0.0010(2)	
$A_{0,-3}$	-0.0024	-0.0049	-0.0017	
$B_{0,-3}$	0.0005	0.0009	-0.0010	
$A_{-3,3}$	-0.0024	0.0024	-0.0017	
$B_{-3,3}$	0.0005	-0.0005	-0.0010	
C	x	y	z	100×B/8π^2(Å^2)
Average	0.0	0.0	0.5	0.89(4)
$A_{1,0}$	0.0	0.0	0.0	
$B_{1,0}$	0.0037(8)	0.0018	-0.0233(4)	
$A_{0,-1}$	0.0	0.0	0.0	
$B_{0,-1}$	-0.0018	-0.0037	-0.0233	
$A_{-1,1}$	0.0	0.0	0.0	
$B_{-1,1}$	-0.0018	0.0018	-0.0233	
Subsystem 2				
$B_{1/3}C_{2/3}$	x	y	z	100×B/8π^2(Å^2)
Average	0.333333	0.666667	-0.0004(3)	0.96(3)
$A_{1,0}$	-0.0075(9)	-0.0037	-0.0266(2)	
$B_{1,0}$	-0.0014(9)	-0.0007	-0.0212(2)	
$A_{0,-1}$	0.0037	0.0075	-0.0266	
$B_{0,-1}$	0.0007	0.0014	-0.0212	
$A_{-1,1}$	0.0037	-0.0037	-0.0266	
$B_{-1,1}$	0.0007	-0.0007	-0.0212	

Table V. Anisotropic thermal parameters of Sc for the second model. $A_{m,n}$ and $B_{m,n}$ are the cosine and sine terms of the Fourier amplitudes with the wave vector $m\boldsymbol{a}_2^*+n\boldsymbol{b}_2^*$

Sc	$100\times U_{11}$	$100\times U_{12}$	$100\times U_{13}$	$100\times U_{22}$	$100\times U_{23}$	$100\times U_{33}$
Average	0.74(1)	0.37	0.00	0.74	0.00	0.85(2)
$A_{1,0}$	-0.20(1)	-0.10	0.08(1)	-0.06(1)	0.04	-0.04(2)
$B_{1,0}$	-0.01(1)	-0.00	-0.04(1)	0.01(2)	-0.02	0.01(1)
$A_{0,-1}$	-0.06	-0.10	-0.04	-0.20	-0.08	-0.04
$B_{0,-1}$	0.01	-0.00	0.02	-0.01	0.04	0.00
$A_{-1,1}$	-0.06	0.04	-0.04	-0.06	0.04	-0.04
$B_{-1,1}$	0.01	0.01	0.02	0.00	-0.02	0.00

Note 1. The anisotropic displacement factor exponent takes the form:

$$-2\pi^2(h^2a^{*2}U_{11}+2hka^*b^*U_{12}+2hla^*c^*U_{13}+k^2b^{*2}U_{22}+2klb^*c^*U_{23}+l^2c^{*2}U_{33}).$$

Note 2. $U_{eq}=B_{eq}/(8\pi^2)=(1/3)[(\boldsymbol{a},\boldsymbol{a})\,a^{*2}U_{11}+(\boldsymbol{b},\boldsymbol{b})\,b^{*2}U_{22}+(\boldsymbol{c},\boldsymbol{c})c^{*2}U_{33}+2(\boldsymbol{a},\boldsymbol{b})a^*b^*U_{12}]$.

Table VI. Interatomic distances (Å) calculated for the second model using the parameters listed in Table IV.

1)$\mathrm{CSc_6}$ octahedral unit

		*
$\mathrm{C}^{(155)}$		1a
$-\mathrm{Sc}^{(155)},\mathrm{Sc}^{(154)},\mathrm{Sc}^{(144)},\mathrm{Sc}^{(7’55)},\mathrm{Sc}^{(7’56)},\mathrm{Sc}^{(7’66)}$	2.293(6)×3, 2.356(5)×3	
$\mathrm{C}^{(167)}$		3d
$-\mathrm{Sc}^{(166)},\mathrm{Sc}^{(156)},\mathrm{Sc}^{(7’68)},\mathrm{Sc}^{(7’78)},\mathrm{Sc}^{(167)},\mathrm{Sc}^{(7’67)}$	2.302(3) ×2, 2.293(3) ×2, 2.303(4), 2.295(5)	
$\mathrm{C}^{(176)}$		3d
$-\mathrm{Sc}^{(176)},\mathrm{Sc}^{(175)},\mathrm{Sc}^{(7’76)},\mathrm{Sc}^{(7’77)},\mathrm{Sc}^{(165)},\mathrm{Sc}^{(7’87)}$	2.350(4) ×2, 2.309(5) ×2, 2.283(5), 2.288(5)	
$\mathrm{C}^{(173)}$		3d
$-\mathrm{Sc}^{(173)},\mathrm{Sc}^{(162)},\mathrm{Sc}^{(7’73)},\mathrm{Sc}^{(7’84)},\mathrm{Sc}^{(172)},\mathrm{Sc}^{(7’74)}$	2.345(4) ×2, 2.288(4) ×2, 2.303(5), 2.281(5)	
$\mathrm{C}^{(127)}$		3d
$-\mathrm{Sc}^{(126)},\mathrm{Sc}^{(116)},\mathrm{Sc}^{(7’28)},\mathrm{Sc}^{(7’27)},\mathrm{Sc}^{(116)},\mathrm{Sc}^{(7’38)}$	2.266(4) ×2, 2.305(4) ×2, 2.275(6), 2.310(5)	
$\mathrm{C}^{(182)}$		3d
$-\mathrm{Sc}^{(182)},\mathrm{Sc}^{(171)},\mathrm{Sc}^{(7’82)},\mathrm{Sc}^{(7’93)},\mathrm{Sc}^{(181)},\mathrm{Sc}^{(7’83)}$	2.315(3) ×2, 2.271(3) ×2, 2.260(4), 2.223(5)	
$\mathrm{C}^{(126)}$		3d
$-\mathrm{Sc}^{(125)},\mathrm{Sc}^{(115)},\mathrm{Sc}^{(7’27)},\mathrm{Sc}^{(7’37)},\mathrm{Sc}^{(126)},\mathrm{Sc}^{(7’26)}$	2.284(3) ×2, 2.332(4) ×2, 2.305(6), 2.278(5)	
$\mathrm{C}^{(156)}$		6e
$-\mathrm{Sc}^{(156)},\mathrm{Sc}^{(7’57)},\mathrm{Sc}^{(155)},\mathrm{Sc}^{(7’56)},\mathrm{Sc}^{(145)},\mathrm{Sc}^{(7’67)}$	2.293(4),2.290(3),2.269(3),2.296(4),2.335(4),2.291(4)	
$\mathrm{C}^{(157)}$		6e
$-\mathrm{Sc}^{(157)},\mathrm{Sc}^{(7’58)},\mathrm{Sc}^{(156)},\mathrm{Sc}^{(7’57)},\mathrm{Sc}^{(146)},\mathrm{Sc}^{(7’68)}$	2.315(4),2.325(4),2.292(4),2.271(3),2.285(4),2.307(5)	
$\mathrm{C}^{(158)}$		6e
$-\mathrm{Sc}^{(158)},\mathrm{Sc}^{(7’59)},\mathrm{Sc}^{(157)},\mathrm{Sc}^{(7’58)},\mathrm{Sc}^{(147)},\mathrm{Sc}^{(7’69)}$	2.276(4),2.306(4),2.299(4),2.275(4),2.330(4),2.343(4)	
$\mathrm{C}^{(168)}$		6e
$-\mathrm{Sc}^{(168)},\mathrm{Sc}^{(7’68)},\mathrm{Sc}^{(157)},\mathrm{Sc}^{(7’69)},\mathrm{Sc}^{(167)},\mathrm{Sc}^{(7’79)}$	2.317(4),2.264(4),2.290(4),2.290(5),2.298(4),2.286(3)	
$\mathrm{C}^{(142)}$		6e
$-\mathrm{Sc}^{(142)},\mathrm{Sc}^{(7’43)},\mathrm{Sc}^{(141)},\mathrm{Sc}^{(7’42)},\mathrm{Sc}^{(131)},\mathrm{Sc}^{(7’53)}$	2.269(3),2.266(3),2.243(3),2.310(4),2.294(3),2.346(4)	

2)Sc-C(<2.4 Å), M(<2.6 Å) M= $\mathrm{B_{1/3}C_{2/3}}$

		*
$\mathrm{Sc}^{(172)}$		1b
$-\mathrm{C}^{(172)},\mathrm{C}^{(173)},\mathrm{C}^{(183)}$	2.303(5)×3	
$-\mathrm{M}^{[782]}$	2.462(8)	
$\mathrm{Sc}^{(155)}$		3d
$-\mathrm{C}^{(155)},\mathrm{C}^{(156)},\mathrm{C}^{(166)}$	2.293(6), 2.269(3) ×2	
$-\mathrm{M}^{[155]},\mathrm{M}^{[144]},\mathrm{M}^{[766]}$	2.472(5), 2.544(5),2.550(5)	
$\mathrm{Sc}^{(165)}$		3d
$-\mathrm{C}^{(165)},\mathrm{C}^{(166)},\mathrm{C}^{(176)}$	2.335(4) ×2, 2.283(5)	
$-\mathrm{M}^{[164]},\mathrm{M}^{[165]},\mathrm{M}^{[776]}$	2.509(4) ×2, 2.502(6)	
$\mathrm{Sc}^{(167)}$		3d
$-\mathrm{C}^{(167)},\mathrm{C}^{(168)},\mathrm{C}^{(178)}$	2.303(4), 2.298(4) ×2	
$-\mathrm{M}^{[167]},\mathrm{M}^{[779]}$	2.306(6),2.529(5)	
$\mathrm{Sc}^{(186)}$		3d
$-\mathrm{C}^{(186)},\mathrm{C}^{(187)},\mathrm{C}^{(197)}$	2.294(3) ×2, 2.275(6)	
$-\mathrm{M}^{[196]},\mathrm{M}^{[797]}$	2.371(5) , 2.520(6)	
$\mathrm{Sc}^{(127)}$		3d
$-\mathrm{C}^{(127)},\mathrm{C}^{(138)},\mathrm{C}^{(128)}$	2.266(4) ×2, 2.305(6)	
$-\mathrm{M}^{[117]},\mathrm{M}^{[718]},\mathrm{M}^{[729]}$	2.367(6), 2.565(5) ×2	
$\mathrm{Sc}^{(158)}$		3d
$-\mathrm{C}^{(169)},\mathrm{C}^{(158)},\mathrm{C}^{(159)}$	2.260(4), 2.276(4) ×2	
$-\mathrm{M}^{[158]},\mathrm{M}^{[148]},\mathrm{M}^{[759]},\mathrm{M}^{[7510]}$	2.490(4), 2.485(5), 2.545(4),2.561(5)	
$\mathrm{Sc}^{(156)}$		6e
$-\mathrm{C}^{(156)},\mathrm{C}^{(157)},\mathrm{C}^{(167)}$	2.293(4), 2.292(4), 2.302(3)	
$-\mathrm{M}^{[156]},\mathrm{M}^{[757]}$	2.338(5), 2.503(4)	
$\mathrm{Sc}^{(157)}$		6e
$-\mathrm{C}^{(157)},\mathrm{C}^{(158)},\mathrm{C}^{(168)}$	2.315(4), 2.299(4), 2.290(4)	
$-\mathrm{M}^{[157]},\mathrm{M}^{[758]},\mathrm{M}^{[769]}$	2.402(4), 2.531(4), 2.515(3)	
$\mathrm{Sc}^{(175)}$		6e
$-\mathrm{C}^{(175)},\mathrm{C}^{(176)},\mathrm{C}^{(186)}$	2.285(4), 2.350(4), 2.269(3)	

-$M^{[174]}$,$M^{[786]}$	2.490(4), 2.505(5)	
$Sc^{(168)}$		6e
-$C^{(168)}$,$C^{(169)}$,$C^{(179)}$	2.317(4), 2.315(3), 2.345(4)	
-$M^{[168]}$,$M^{[769]}$,$M^{[7710]}$	2.364(3), 2.577(3),2.493(4)	
$Sc^{(185)}$		6e
-$C^{(185)}$,$C^{(186)}$,$C^{(196)}$	2.330(4), 2.243(3), 2.284(4)	
-$M^{[184]}$,$M^{[194]}$,$M^{[195]}$,$M^{[796]}$,$M^{[7106]}$	2.569(4),2.591(4),2.459(4),2.556(4),2.557(4)	
$Sc^{(7'38)}$		1c
-$C^{(127)}$,$C^{(137)}$,$C^{(138)}$	2.310(5) ×3	
-$M^{[1'16]}$,$M^{[1'17]}$,$M^{[1'27]}$,$M^{[7'28]}$	2.592(7) ×3, 2.283(8)	
$Sc^{(7'55)}$		3d
-$C^{(144)}$,$C^{(154)}$,$C^{(155)}$	2.296(4) ×2, 2.356(5)	
-$M^{[1'43]}$,$M^{[7'44]}$,$M^{[7'54]}$	2.500(6), 2.555(5) ×2	
$Sc^{(7'65)}$		3d
-$C^{(154)}$,$C^{(165)}$,$C^{(164)}$	2.291(4) ×2, 2.295(5)	
-$M^{[1'53]}$,$M^{[7'64]}$	2.505(5) , 2.337(5)	
$Sc^{(7'87)}$		3d
-$C^{(187)}$,$C^{(186)}$,$C^{(176)}$	2.266(3) ×2, 2.288(5)	
-$M^{[1'75]}$,$M^{[1'85]}$,$M^{[1'86]}$,$M^{[7'86]}$,$M^{[7'87]}$,$M^{[7'97]}$	2.550(5) 2.544(4) ×2, 2.490(4) ×2 ,2.474(4)	
$Sc^{(7'79)}$		3d
-$C^{(168)}$,$C^{(178)}$,$C^{(179)}$	2.286(3) ×2, 2.281(5)	
-$M^{[1'68]}$, $M^{[1'78]}$, $M^{[7'79]}$	2.544(4) ×2, 2.409(5)	
$Sc^{(7'73)}$		3d
-$C^{(173)}$,$C^{(172)}$,$C^{(162)}$	2.288(4) ×2, 2.223(5)	
-$M^{[1'60]}$,$M^{[1'70]}$, $M^{[7'71]}$, $M^{[7'82]}$	2.581(5) 2.594(5), 2.520(5), 2.557(6)	
$Sc^{(7'59)}$		3d
-$C^{(148)}$,$C^{(158)}$,$C^{(159)}$	2.278(5), 2.306(4) ×2	
-$M^{[1'48]}$,$M^{[7'49]}$	2.485(6) , 2.547(5)	
$Sc^{(7'54)}$		6e
-$C^{(143)}$,$C^{(154)}$,$C^{(153)}$	2.309(5), 2.290(3), 2.271(3)	
-$M^{[1'42]}$,$M^{[1'41]}$,$M^{[7'43]}$,$M^{[7'42]}$,$M^{[7'53]}$	2.555(4), 2.520(4),2.597(4),2.570(5),2.445(4)	
$Sc^{(7'53)}$		6e
-$C^{(142)}$,$C^{(153)}$,$C^{(152)}$	2.346(4), 2.325(4), 2.275(4)	
-$M^{[1'41]}$,$M^{[1'40]}$,$M^{[7'41]}$,$M^{[7'52]}$	2.592(3), 2.508(4),2.578(4),2.427(4)	
$Sc^{(7'64)}$		6e
-$C^{(153)}$,$C^{(164)}$,$C^{(163)}$	2.307(5), 2.293(3), 2.264(4)	
-$M^{[1'51]}$,$M^{[7'63]}$	2.526(4), 2.338(5)	
$Sc^{(7'37)}$		6e
-$C^{(136)}$,$C^{(126)}$,$C^{(137)}$	2.310(4), 2.332(5), 2.305(4)	
-$M^{[1'15]}$,$M^{[1'26]}$,$M^{[7'27]}$	2.499(4), 2.538(4),2.347(4)	
$Sc^{(7'85)}$		6e
-$C^{(174)}$,$C^{(184)}$,$C^{(185)}$	2.290(5), 2.271(3),2.343(4)	
-$M^{[1'83]}$,$M^{[7'84]}$	2.513(5), 2.399(4)	

3)M-M (<1.6Å)	M= $B_{1/3}C_{2/3}$	*
$M^{[755]}$		1a
- $M^{[154]}$, $M^{[144]}$, $M^{[143]}$	1.535(3) ×3	
$M^{[782]}$		1b
- $M^{[181]}$, $M^{[171]}$, $M^{[170]}$	1.542(3) ×3	
$M^{[728]}$		1c
- $M^{[127]}$, $M^{[117]}$, $M^{[116]}$	1.508(3) ×3	
$M^{[767]}$		3d
- $M^{[166]}$, $M^{[156]}$, $M^{[155]}$	1.524(3) ×2, 1.515(4)	
$M^{[776]}$		3d
- $M^{[165]}$, $M^{[164]}$, $M^{[175]}$	1.547(4) ×2, 1.544(5)	
$M^{[779]}$		3d
- $M^{[178]}$, $M^{[168]}$, $M^{[167]}$	1.514(1) ×2, 1.505(3)	
$M^{[797]}$		3d
- $M^{[186]}$, $M^{[185]}$, $M^{[96]}$	1.529(1) ×2, 1.530(4)	
$M^{[794]}$		3d
- $M^{[193]}$, $M^{[183]}$, $M^{[182]}$	1.536(2) ×2, 1.572(8)	

$M^{[749]}$ - $M^{[138]}$, $M^{[137]}$, $M^{[148]}$	1.539(4) ×2, 1.547(4)	3d
$M^{[756]}$ - $M^{[144]}$, $M^{[145]}$, $M^{[155]}$	1.547(4), 1.564(7), 1.5236(6)	6e
$M^{[757]}$ - $M^{[145]}$, $M^{[146]}$, $M^{[156]}$	1.523(2), 1.527(2), 1.510(3)	6e
$M^{[758]}$ - $M^{[146]}$, $M^{[147]}$, $M^{[157]}$	1.551(5), 1.539(4), 1.515(2)	6e
$M^{[759]}$ - $M^{[147]}$, $M^{[148]}$, $M^{[158]}$	1.551(6), 1.538(2), 1.531(2)	6e
$M^{[768]}$ - $M^{[156]}$, $M^{[157]}$, $M^{[167]}$	1.514(3), 1.505(2), 1.511(3)	6e
$M^{[769]}$ - $M^{[157]}$, $M^{[158]}$, $M^{[168]}$	1.523(2), 1.538(4), 1.544(5)	6e
$M^{[772]}$ - $M^{[160]}$, $M^{[161]}$, $M^{[171]}$	1.541(3), 1.531(4), 1.539(4)	6e
$M^{[786]}$ - $M^{[174]}$, $M^{[175]}$, $M^{[185]}$	1.547(4), 1.533(2), 1.542(3)	6e
$M^{[796]}$ - $M^{[184]}$, $M^{[185]}$, $M^{[195]}$	1.547(4), 1.565(7), 1.534(3)	6e
$M^{[727]}$ - $M^{[115]}$, $M^{[116]}$, $M^{[126]}$	1.517(3), 1.510(2), 1.531(3)	6e
$M^{[155]}$ - $M^{[756]}$, $M^{[766]}$, $M^{[767]}$	1.5236(6) ×2, 1.515(4)	3d
$M^{[154]}$ - $M^{[766]}$, $M^{[765]}$, $M^{[755]}$	1.547(4) ×2, 1.535(3)	3d
$M^{[167]}$ - $M^{[768]}$, $M^{[778]}$, $M^{[779]}$	1.511(3) ×2, 1.505(3)	3d
$M^{[175]}$ - $M^{[787]}$, $M^{[786]}$, $M^{[776]}$	1.533(2) ×2, 1.544(5)	3d
$M^{[181]}$ - $M^{[793]}$, $M^{[792]}$, $M^{[782]}$	1.539(4) ×2, 1.542(3)	3d
$M^{[126]}$ - $M^{[727]}$, $M^{[738]}$, $M^{[737]}$	1.531(3) ×2, 1.530(4)	3d
$M^{[182]}$ - $M^{[783]}$, $M^{[793]}$, $M^{[794]}$	1.541(3) ×2, 1.572(8)	3d
$M^{[148]}$ - $M^{[759]}$, $M^{[7510]}$, $M^{[749]}$	1.538(2)×2, 1.547(4)	3d
$M^{[116]}$ - $M^{[717]}$, $M^{[727]}$, $M^{[728]}$	1.510(2) ×2, 1.508(3)	3d
$M^{[156]}$ - $M^{[757]}$, $M^{[767]}$, $M^{[768]}$	1.510(3), 1.524(3), 1.514(3)	6e
$M^{[157]}$ - $M^{[758]}$, $M^{[768]}$, $M^{[769]}$	1.515(2), 1.505(2), 1.523(2)	6e
$M^{[158]}$ - $M^{[759]}$, $M^{[769]}$, $M^{[7610]}$	1.531(2), 1.538(4), 1.536(2)	6e
$M^{[165]}$ - $M^{[776]}$, $M^{[777]}$, $M^{[766]}$	1.547(4), 1.523(2), 1.564(7)	6e
$M^{[161]}$ - $M^{[762]}$, $M^{[772]}$, $M^{[777]}$	1.544(5), 1.531(4), 1.514(1)	6e
$M^{[176]}$ - $M^{[777]}$, $M^{[787]}$, $M^{[788]}$	1.527(2), 1.547(4), 1.551(5)	6e
$M^{[185]}$ - $M^{[786]}$, $M^{[796]}$, $M^{[797]}$	1.542(3), 1.565(7), 1.529(1)	6e
$M^{[187]}$ - $M^{[788]}$, $M^{[798]}$, $M^{[799]}$	1.539(4), 1.547(4), 1.551(6)	6e
$M^{[115]}$ - $M^{[716]}$, $M^{[726]}$, $M^{[727]}$	1.539(4), 1.534(3), 1.517(3)	6e

Symmetry codes in the first subsystem: (1pq)x+p-5,y+q-5,z (7’pq)-x+p-5,-y+q-5,1-z

Symmetry codes in the second subsystem: [1pq]x+p-5,y+q-5,z [7pq]-x+p-5,-y+q-5,-z [1’pq]x+p-5,y+q-5,z+1 [7’pq]-x+p-5,-y+q-5,1-z

*Wyckoff notation in a large superlattice unit cell, *A*=23.710(9) and *c*=6.703(2)Å, with space group P3m1.