

## Supplemental data

### Extinction and final parameters at 430K

$\Delta\rho_A$  is the height of maximum peaks along  $\langle 100 \rangle$  directions at  $0.8\text{\AA}$  from Ce in residual density distribution. Details are same as Table 2.

Refinement	Degeneracy	(A)SPH	(B) without 5d	(C) $5d(j=5/2)\Gamma_8$	(D) $5d(j=3/2)\Gamma_8$
$R_1$ (%)		1.248	1.164	1.132	1.138
$R_2$ (%)		1.675	1.539	1.443	1.455
Ce					
$U_{11}$		856(2)	847(2)	847(2)	847(2)
$b_1$		694(2)	701(2)	701(2)	701(2)
$n$ (4f $j=5/2 \Gamma_8$ )	4	1/6	0.00	0.10(14)	0.12(19)
$n$ (4f $j=5/2 \Gamma_7$ )	2	1/6	0.48(10)	0.61(23)	0.48(28)
$n$ (5d $j=5/2 \Gamma_8$ )	4	-	-	1	-
$n$ (5d $j=3/2$ )	4	-	-	-	1
$\kappa$ (4f $j=5/2 \Gamma_8$ )	4	-	-	1.28(23)	1.52(29)
$\kappa$ (4f $j=5/2 \Gamma_7$ )	2	-	1.65(22)	1.45(14)	1.42(31)
$\kappa$ (5p $j=3/2$ )	4	-	0.89(4)	0.89(4)	0.89(4)
$\kappa$ (5d $j=5/2 \Gamma_8$ )	4	-	-	1.12(11)	-
$\kappa$ (5d $j=3/2$ )	4	-	-	-	1.07(12)
$q_{1111}$		-	-0.6(3)	-0.3(6)	-0.1(8)
$q_{1122}$		-	1.9(10)	2.6(18)	1.2(22)
$\Delta\rho_A$ ( $e\text{\AA}^{-3}$ )		0.65	0.74	0.59	0.71
Valence of Ce		+3.00(-)	+3.04(20)	-1.62(72)	-1.44(94)
B					
$z$		0.30085(29)	0.30192(414)	0.30223(240)	0.30233(247)
$U_{11}$		616(9)	612(7)	613(7)	613(7)
$U_{33}$		380(12)	368(9)	366(9)	366(9)
$b_1$		963(13)	971(11)	968(10)	969(10)
$b_3$		1563(49)	1612(40)	1622(39)	1622(39)
$n$ (2s)	1	2.00	2.00	2.00	2.00
$n$ (2p <sub>x</sub> )= $n$ (2p <sub>y</sub> )	2	1/2	0.46(8)	0.0	0.04(8)
$n$ (2p <sub>z</sub> )	1	1/2	0.59(16)	0.73(12)	0.68(22)
$\kappa$ (2s)	1	-	0.96(5)	0.99(4)	0.98(5)
$\kappa$ (2p <sub>x</sub> )= $\kappa$ (2p <sub>y</sub> )	2	-	0.71(9)	-	1.00
$\kappa$ (2p <sub>z</sub> )	1	-	0.92(18)	0.90(10)	0.90(15)
$c_{311}$		0.0	-2.0(55)	-1.3(57)	-0.8(58)
$c_{333}$		0.0	9.3(116)	10.7(131)	12.0(133)
$q_{1111}$		0.0	-12.6(80)	-10.9(78)	-11.5(79)
$q_{3333}$		0.0	-135.3(352)	-126.8(359)	-132.3(365)
$q_{1122}$		0.0	-89.2(404)	-84.1(39)	-85.1(393)
$q_{1133}$		0.0	257.8(649)	246.1(645)	251.0(649)
Extinction					
$Y_{11}$		11.0(5)	12.5(6)	11.3(5)	11.6(8)
$Y_{22}$		6.9(9)	8.4(11)	9.3(11)	9.1(12)
$Y_{33}$		12.4(10)	14.3(12)	13.6(10)	13.4(13)
$Y_{12}$		-0.8(5)	-1.1(5)	-1.3(5)	-1.2(5)

$Y_{13}$	1.0(4)	1.1(5)	0.8(4)	0.8(4)
$Y_{23}$	1.3(8)	1.8(9)	1.7(8)	1.8(8)
$\Delta\rho_{\max}$ ( $e\text{\AA}^{-3}$ )	0.88	0.75	0.59	0.71
$\Delta\rho_{\text{Boron}}$ ( $e\text{\AA}^{-3}$ )	-0.68	-0.50	-0.36	-0.41