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New cerium cobalt borocarbide synthesized from eutectic metal flux mixture

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Supporting Information

Table S1: Atomic coordinates, site occupancies, and equivalent isotropic displacement parameters for $Ce_{10}Co_{2.64}B_{11.70}C_{10}$.

Figure S1: Ordered part of $Ce_{10}Co_{2.64}B_{11.70}C_{10}$ structure viewed down *a*-axis, with atom labels

Figure S2: Disordered region of $Ce_{10}Co_{2.64}B_{11.70}C_{10}$ structure with atom labels, viewed down *c*-axis

Table S1. Atomic coordinates (x 10^4) site occupancies, and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for $Ce_{10}Co_{2.64}B_{11.70}C_{10}$. All atoms are on 2*i* Wyckoff sites. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)	occ*
Ce(1)	3613(1)	5824(1)	980(1)	9(1)	
Ce(2)	7600(1)	7798(1)	987(1)	9(1)	
Ce(3)	-383(1)	3816(1)	1030(1)	8(1)	
Ce(4)	1600(1)	9772(1)	983(1)	9(1)	
Ce(5)	5562(1)	1766(1)	978(1)	12(1)	
Ce(6)	8971(1)	7581(1)	3568(1)	14(1)	
Ce(7)	734(1)	11555(1)	3564(1)	14(1)	
Ce(8)	4800(1)	9415(1)	3063(1)	10(1)	
Ce(9)	2862(1)	5445(1)	3565(1)	14(1)	
Ce(10)	6847(1)	3695(1)	3575(1)	15(1)	
Co(1)	4109(1)	8147(1)	4999(1)	10(1)	
Co(2)	6850(1)	9114(1)	5003(1)	10(1)	
B(1)	12168(6)	8722(6)	4016(4)	12(1)	
C(1)	11768(5)	8244(6)	2859(3)	14(1)	
B(2)	-1003(6)	2729(6)	-1945(4)	12(1)	
C(2)	-572(5)	3232(5)	-865(4)	12(1)	
B(3)	-2373(6)	10685(6)	4022(4)	11(1)	
C(3)	-2225(6)	10475(6)	2864(3)	14(1)	
B(4)	-1644(6)	10899(6)	1959(4)	13(1)	
C(4)	1419(5)	9233(5)	-881(4)	13(1)	
B(5)	3932(6)	2439(6)	4014(4)	12(1)	
C(5)	3700(5)	2354(6)	2858(3)	14(1)	
B(6)	7111(6)	7228(6)	-1950(4)	12(1)	
C(6)	7388(5)	7219(5)	-874(4)	13(1)	
B(7)	5863(6)	6969(6)	4018(3)	11(1)	
C(7)	5882(5)	6351(5)	2871(3)	13(1)	
B(8)	6494(6)	5396(6)	1962(4)	12(1)	
C(8)	3415(5)	5278(5)	-890(3)	12(1)	
C(9)	5413(5)	1191(5)	-921(3)	10(1)	
B(9)	9042(6)	10319(6)	4999(4)	12(1)	
B(10)	5326(6)	5958(6)	4999(4)	12(1)	
B(21)	7234(7)	6660(7)	5003(4)	10(2)	0.82(3)
B(22)	8353(7)	12229(7)	5003(4)	14(2)	0.88(3)
Co(21)	232(4)	14055(4)	4999(2)	13(1)	0.205(4)
Co(22)	9051(4)	4780(4)	5006(2)	13(1)	0.197(4)
Co(23)	7955(9)	6187(9)	5007(5)	25(2)	0.122(5)
Co(24)	8805(9)	12947(10)	4998(5)	21(2)	0.112(5)
C(21)	8824(15)	5665(15)	5010(9)	21(4)	0.46(3)
C(22)	-686(15)	13817(15)	5013(9)	21(3)	0.46(3)

* Site occupancy is 100% unless otherwise stated. Atoms in disordered building block are in blue font.

Figure S1. Ordered part of $Ce_{10}Co_{2.64}B_{11.70}C_{10}$ structure viewed down a-axis, with atom labels (see table S1).

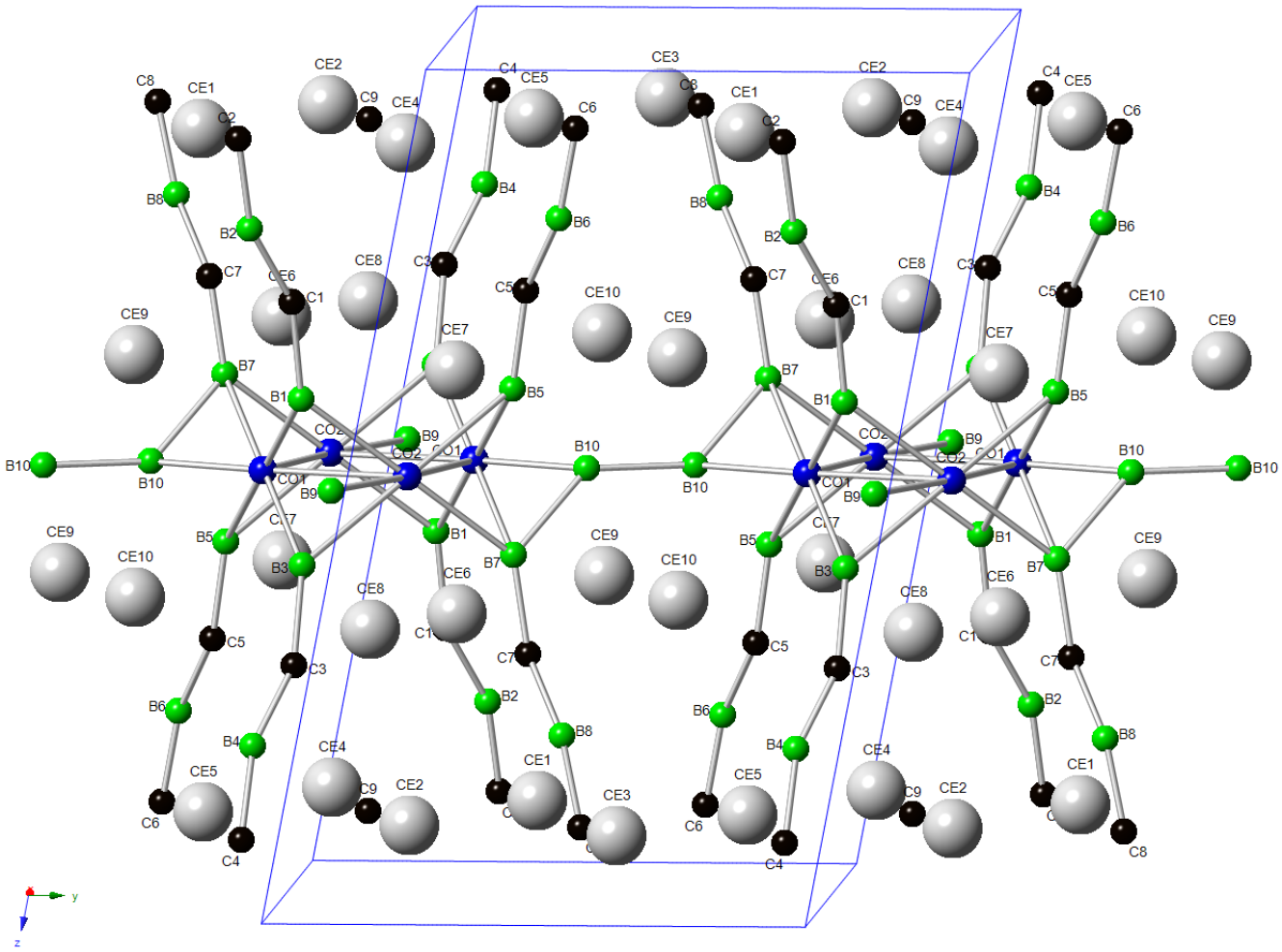

Figure S2. Disordered region of $Ce_{10}Co_{2.64}B_{11.70}C_{10}$ structure with atom labels (see table S1), viewed down c-axis.