Supporting Information

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1. Computational details

We have extensively explored the structures of SrB_xC_{10-x} (x=1-9) at pressures of 0-20 GPa. The formation enthalpy is defined as $\Delta H/11 = H(SrB_xC_{10-x}) - H(Sr) - xH(B) - (10-x)H(C)$ in unit of eV/atom. $H(SrB_xC_{10-x})$ is the enthalpy of SrB_xC_{10-x}. H(Sr), H(B) and H(C) are the enthalpies of elemental Sr, B and C solids, respectively. The *Fm*-3*m* and *Im*-3*m* phases of elemental Sr (phase transition pressure is 5.7 GPa), the *R*-3*m* phase of elemental B and the *Fd*-3*m* structure of elemental C are used in the calculation. In addition, the *C*2/*m* and $P6_3/mmc$ SrB (phase transition pressure is 7.3 GPa), *Immm* SrB_2, *R*-3*m* SrB_4, *Pm*-3*m* SrB_6, *I*4/*mmm* and *C*2/*m* SrC_2 (phase transition pressure is 6.3 GPa) are used to calculate the synthesis pathways. All DFT-GGA calculations were performed for SrB_5C_5, SrB_7C_3, SrB_8C_2, and SrB_9C compounds with atoms numbers of 11, 22, 44, and 44, respectively, which are primitive cells.

2. The COHP curves and ELF distributions.

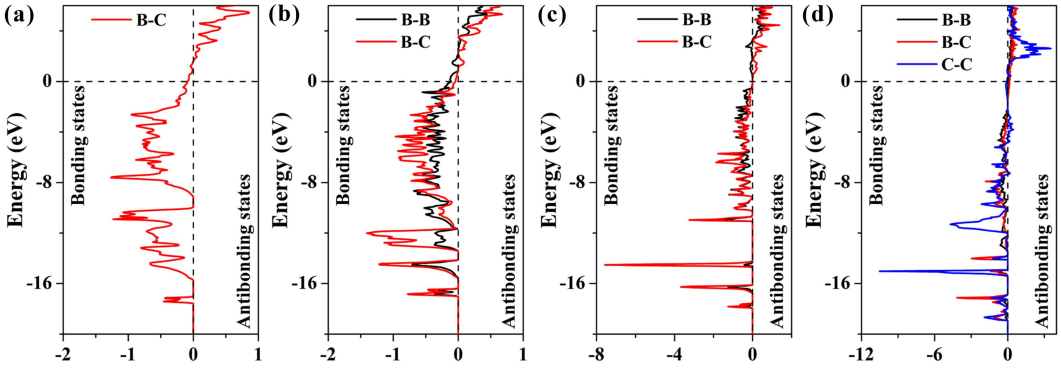

Fig. S1 The COHP curves at 0 GPa for (a) SrB_5C_5, (b) SrB_7C_3 and (d) SrB_9C using PBE functional, and (c) SrB_8C_2 by HSE06 functional.

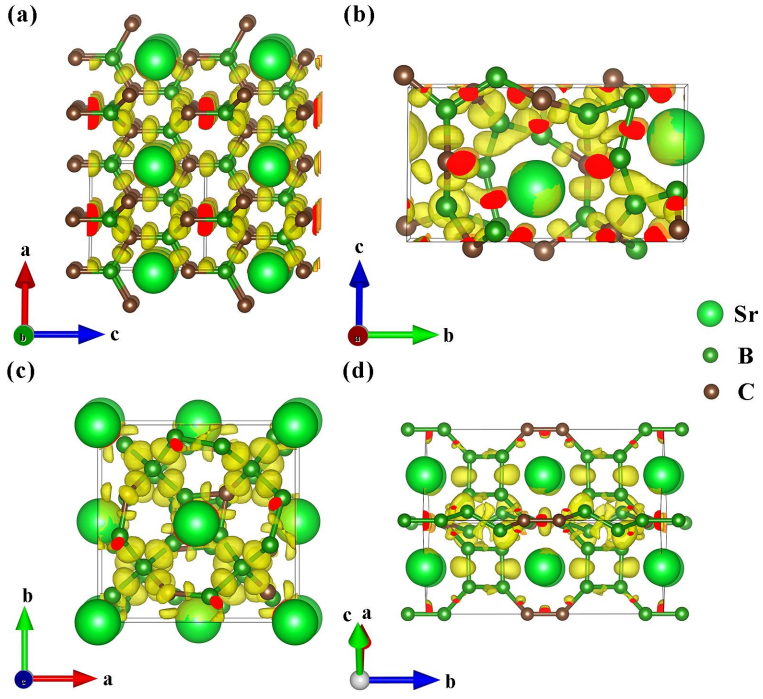

Fig. S2 The ELF distributions for (a) SrB_5C_5, (b) SrB_7C_3, (c) SrB_8C_2 and (d) SrB_9C at ambient pressure (The yellow isosurface represents an ELF value of 0.80).

3. The phonon dispersion curves.

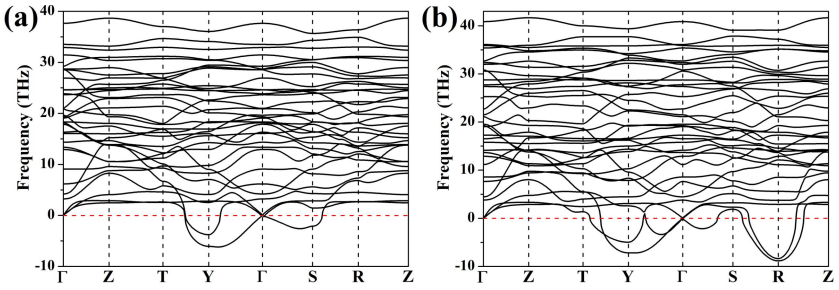

Fig. S3 The phonon dispersion curves for SrB_5C_5 at (a) 0 GPa and (b) 20 GPa.

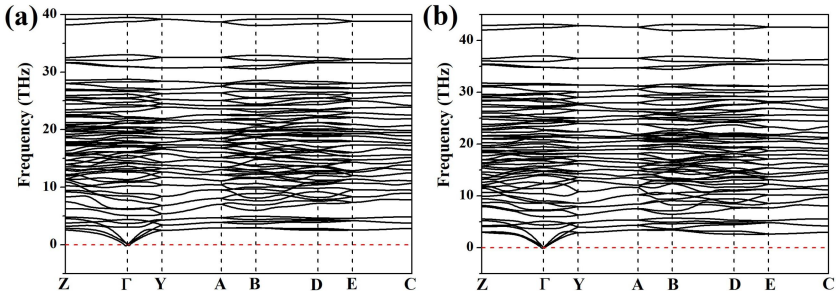

Fig. S4 The phonon dispersion curves for SrB_7C_3 at (a) 0 GPa and (b) 20 GPa.

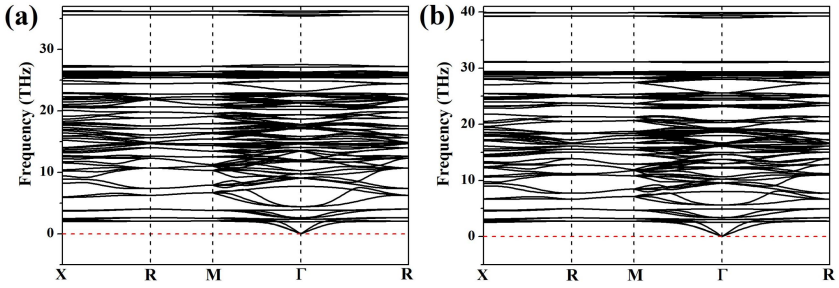

Fig. S5 The phonon dispersion curves for SrB_8C_2 at (a) 0 GPa and (b) 20 GPa.

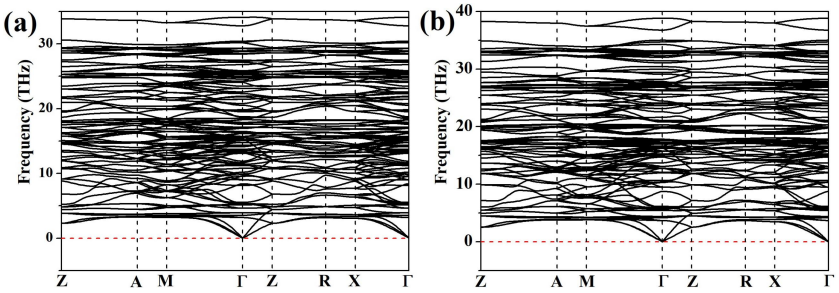

Fig. S6 The phonon dispersion curves for SrB_9C at (a) 0 GPa and (b) 20 GPa.

4. The electronic band structure, transport properties and *ZT* values for SrB_8C_2 at 20 GPa.

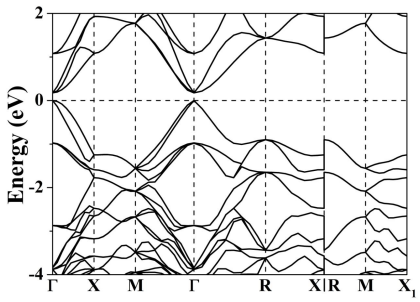

Fig. S7 The electronic band structure of SrB_8C_2 calculated by HSE06 functional at 20 GPa (the bandgap is 0.17 eV, and this value is used to calculate the transport properties).

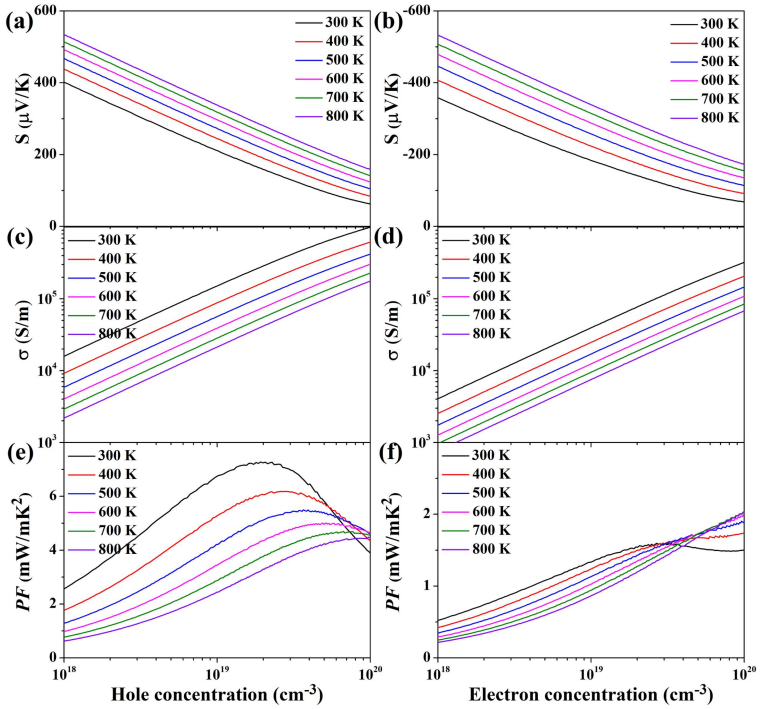

Fig. S8 The transport properties of SrB_8C_2 as a function of carrier concentration between 300 and 800 K at 20 GPa. (a, b) Seebeck coefficients, (c, d) electrical conductivity and (e, f) power factor.

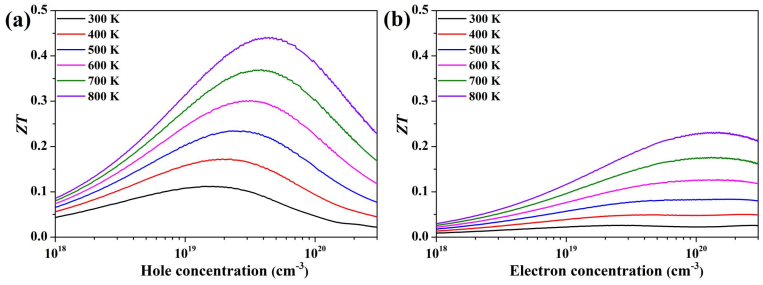

Fig. S9 The (a) *p*-type and (b) *n*-type *ZT* values for SrB_8C_2 between 300 and 800 K at 20 GPa.

5. The detailed structure information and the possible synthesis pathways for SrB_5C_5, SrB_7C_3, SrB_8C_2 and SrB_9C.

Table S1 Detailed crystal structure information for SrB_5C_5, SrB_7C_3, SrB_8C_2 and SrB_9C at ambient pressure.

	Space group	Volume per unit	Lattice parameters		Atomic positions
SrB_5C_5	*Cmm*2	100.0 Å^3	*a* = 8.109 Å, *b* = 5.173 Å *c* = 4.766 Å *α* = *β* = *γ* = 90.0°	Sr	2*a* (0,0,0.58356)
				B	4*c* (0.25,0.25,0.19784)
				B	2*b* (0,0.5,0.20458)
				B	4*d* (0.67644,0,0.71311)
				C	4*c* (0.25,0.25,0.8757)
				C	2*b* (0,0.5,0.8801)
				C	4*d* (0.67653,0,0.36699)
SrB_7C_3	$P2_1$	95.3 Å^3	*a* = 5.114 Å *b* = 8.216 Å *c* = 4.898 Å *α* = *γ* = 90.0° *β* = 112.12°	Sr	2*a* (0.59367,0.46204,0.33407)
				B	2*a* (0.79982,0.6514,0.82655)
				B	2*a* (0.96201,0.31936,0.06623)
				B	2*a* (0.88196,0.13853,0.85647)
				B	2*a* (0.57058,0.13715,0.21969)
				B	2*a* (0.61191,0.82162,0.23853)
				B	2*a* (0.84074,0.97401,0.32316)
				B	2*a* (0.91586,0.76771,0.54251)
				C	2*a* (0.86218,0.14404,0.51885)
				C	2*a* (0.35779,0.73361,0.04503)
				C	2*a* (0.99374,0.98445,0.08073)
SrB_8C_2	*Pa*-3	98.2 Å^3	*a* = *b* = *c* = 7.325 Å *α* = *β* = *γ* = 90.0°	Sr	4*a* (0,0,0)
				B	24*d* (0.62818,0.60976,0.43442)
				B	8*c* (0.77309,0.77309,0.77309)
				C	8*c* (0.64678,0.64678,0.64678)
SrB_9C	*P*4/*nnc*	97.6 Å^3	*a* = *b* = 5.981 Å *c* = 10.912 Å *α* = *β* = *γ* = 90.0°	Sr	4*c* (0,0.5,0)
				B	16*k* (0.90284,0.80307,0.18249)
				B	16*k* (0.40453,0.30215,0.82196)
				B	4*e* (0,0,0.92363)
				C	4*e* (0,0,0.57366)

Table S2 Formation enthalpies of SrB_5C_5, SrB_7C_3, SrB_8C_2 and SrB_9C within different synthesis pathways at 20 GPa.

	Synthesis pathways	ΔH with respect to diamond carbon (meV/atom)
SrB_5C_5	Sr+5B+5C	-16
	SrB+4B+5C	-52
	SrB_2+3B+5C	-129
	SrB_4+B+5C	-197
	SrC_2+5B+3C	-74
	(SrB+SrC_2+9B+8C)/2	-127
	(SrB_2+SrC_2+8B+8C)/2	-203
	(SrB_4+SrC_2+6B+8C)/2	-271
	(SrB_6+SrC_2+8B+8C)/2	-444
SrB_7C_3	Sr+7B+3C	-111
	SrB+6B+3C	43
	SrB_2+5B+3C	-34
	SrB_4+3B+3C	-102
	SrB_6+B+3C	-275
	SrC_2+7B+C	21
	(SrB+SrC_2+13B+4C)/2	64
	(SrB_2+SrC_2+12B+4C)/2	-13
	(SrB_4+SrC_2+10B+4C)/2	-80
	(SrB_6+SrC_2+8B+4C)/2	-254
SrB_8C_2	Sr+8B+2C	-106
	SrB+7B+2C	37
	SrB_2+6B+2C	-39
	SrB_4+4B+2C	-107
	SrB_6+2B+2C	-28
	SrC_2+8B	15
	(SrB+SrC_2+15B+2C)/2	52

	$(SrB_2+SrC_2+14B+2C)/2$	-24
	$(SrB_4+SrC_2+12B+2C)/2$	-92
	$(SrB_6+SrC_2+10B+2C)/2$	-265
SrB_9C	Sr+9B+C	-95
	SrB+8B+C	26
	SrB_2+7B+C	-50
	SrB_4+5B+C	-118
	SrB_6+3B+C	-291
	$(SrB+SrC_2+17B)/2$	31
	$(SrB_2+SrC_2+16B)/2$	46
	$(SrB_4+SrC_2+14B)/2$	-114
	$(SrB_6+SrC_2+12B)/2$	-286

6. The calculated elastic constants, moduli and Bader charges for SrB_7C_3, SrB_8C_2 and SrB_9C.

Table S3 The calculated elastic constants (C_{ij}), bulk modulus (B), shear modulus (G), Young's modulus (Y), Pugh ratio (G/B) and simulated hardness values (H_v) by employing three different empirical model for SrB_7C_3, SrB_8C_2 and SrB_9C compounds at 20 GPa. The units of C_{ij}, B, G, Y, and H_v are GPa.

SrB_7C_3	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	C_{15}
	505.5	576.0	549.0	236.8	212.6	231.9	138.4	161.0	139.6	51.6
	C_{25}	C_{35}	C_{46}	B	G	Y	G/B	H_v^{Chen}	H_v^{Tian}	H_v^{Teter}
	8.9	-11.3	30.1	277.7	212.7	508.4	0.77	30.7	30.2	32.1
SrB_8C_2	C_{11}	C_{44}	C_{12}	B	G	Y	G/B	H_v^{Chen}	H_v^{Tian}	H_v^{Teter}
	497.2	206.6	140.0	259.1	194.9	467.4	0.75	28.3	27.8	29.4
SrB_9C	C_{11}	C_{33}	C_{44}	C_{66}	C_{12}	C_{13}				
	466.7	655.6	216.2	219.2	165.8	106.9				
				B	G	Y	G/B	H_v^{Chen}	H_v^{Tian}	H_v^{Teter}
				259.7	207.7	491.9	0.80	31.9	31.2	31.4

Table S4 The Bader charges for SrB_7C_3, SrB_8C_2 and SrB_9C compounds at ambient pressure.

	Atom	Atom numbers	Charge value (e)	δ (e)
SrB_7C_3	Sr	2	8.57	+1.43
	B	14	2.25	+0.75
	C	6	6.22	-2.22
SrB_8C_2	Sr	4	8.45	+1.55
	B	32	2.57	+0.43
	C	8	6.48	-2.47
SrB_9C	Sr	4	8.60	+1.40
	B	36	2.98	+0.02
	C	4	5.59	-1.59

7. The effective mass, elastic constant, DP constant and relaxation time for SrB_8C_2.

Table S5 The corresponding effective mass m^*, elastic constant C and DP constant E at 0 GPa are listed.

Carrier type	$\lvert m^*\rvert/m_0$	C (eV/Å^3)	$\lvert E\rvert$ (eV per strain)
Electron	0.76	10.6	23.94
Hole	1.66	10.6	25.55

Table S6 The carrier relaxation time for the SrB_8C_2 at 0 GPa.

		300 K	400 K	500 K	600 K	700 K	800 K
τ (10^{-14} s)	CBM	2.97	1.93	1.38	1.05	0.83	0.68
	VBM	8.41	5.46	3.91	2.98	2.36	1.93

Table S7 The corresponding effective mass m^*, elastic constant C and DP constant E at 20 GPa are listed.

Carrier type	$\lvert m^*\rvert/m_0$	C (eV/Å^3)	$\lvert E\rvert$ (eV per strain)
Electron	0.79	14.6	25.38
Hole	1.52	14.6	27.70

Table S8 The carrier relaxation time for the SrB_8C_2 at 20 GPa.

		300 K	400 K	500 K	600 K	700 K	800 K
τ (10^{-14} s)	CBM	4.17	2.71	1.94	1.47	1.17	0.96
	VBM	9.36	6.08	4.35	3.31	2.63	2.15