SUPPLEMENTARY INFORMATION

Synthesis and chemistry of the open-cage cobaltaheteroborane cluster $[\{(\eta^5\text{-}C_5Me_5)Co\}_2B_2H_2Se_2]$: A combined experimental and theoretical study

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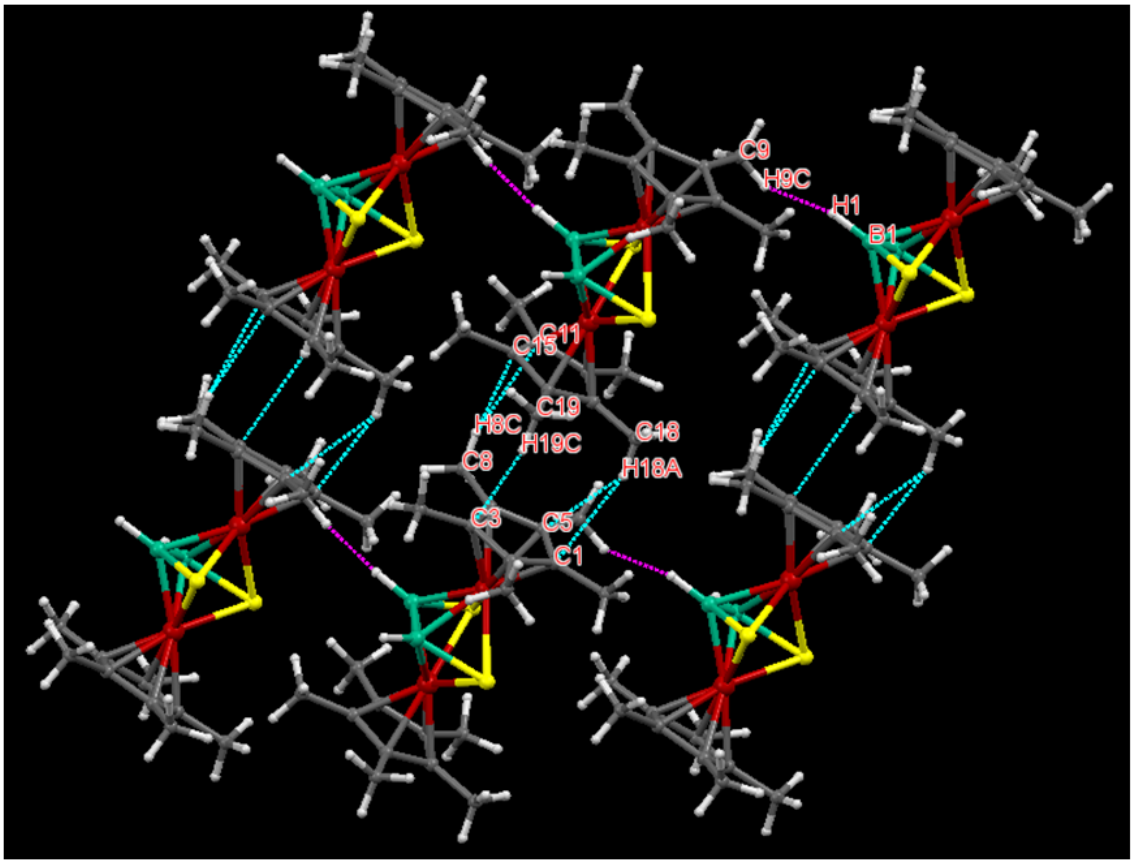

Fig. S1. Illustation of 2D packing view of **1** along *b* axis; Color code: C: dark gray; Co: scarlet; B: green; Se: yellow and H: white.

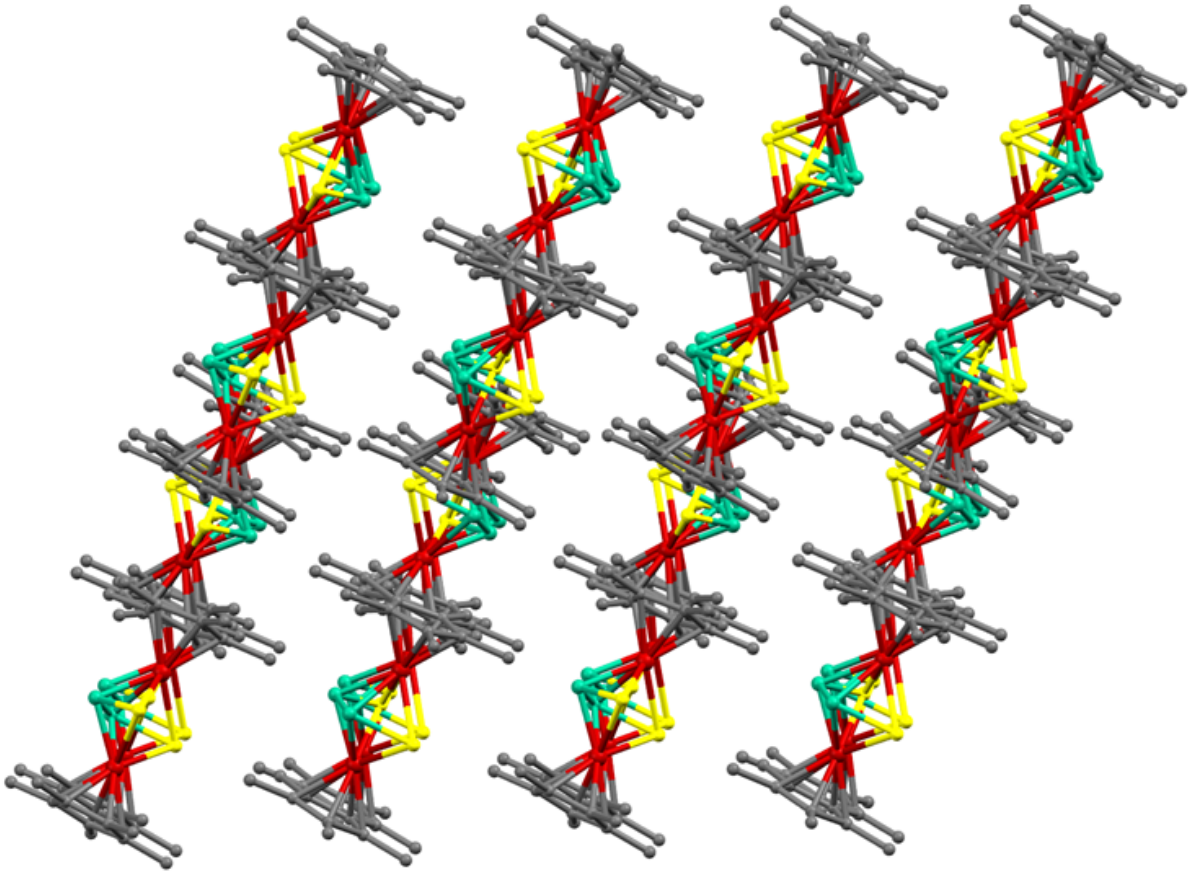

Fig. S2. 3D architecture in **1** parallel to *a*-axis, color code: C: dark gray; Co: scarlet; B: green; and Se: yellow (hydrogen atoms, are removed for clarity).

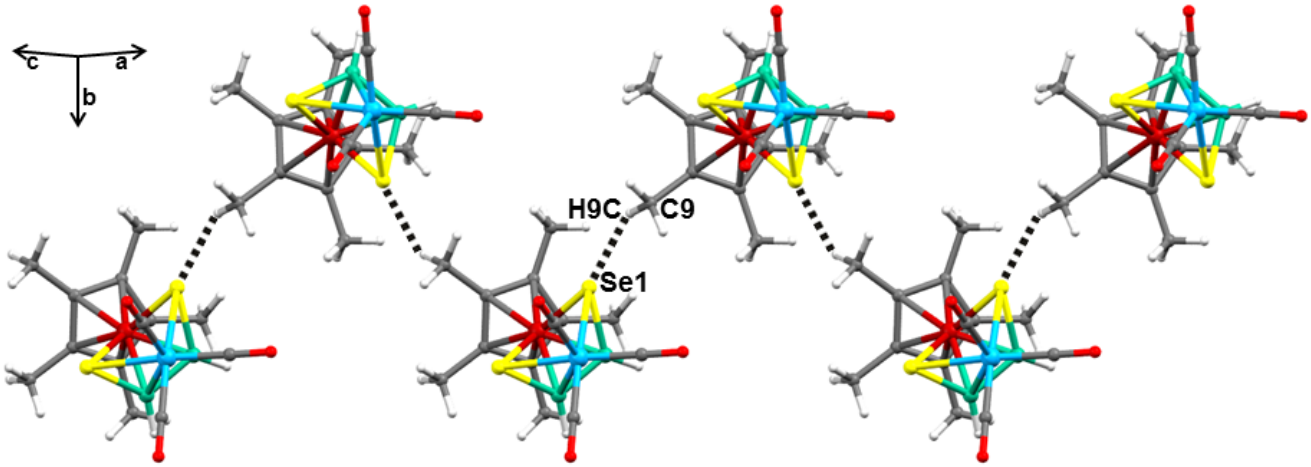

Fig. S3. Vidualization of intermolecular C-H···Se interaction forming an infinite 1D chain in **2**.

Color code: Fe: cyan; C: dark gray; Co: scarlet; B: green; O: red and H: white.

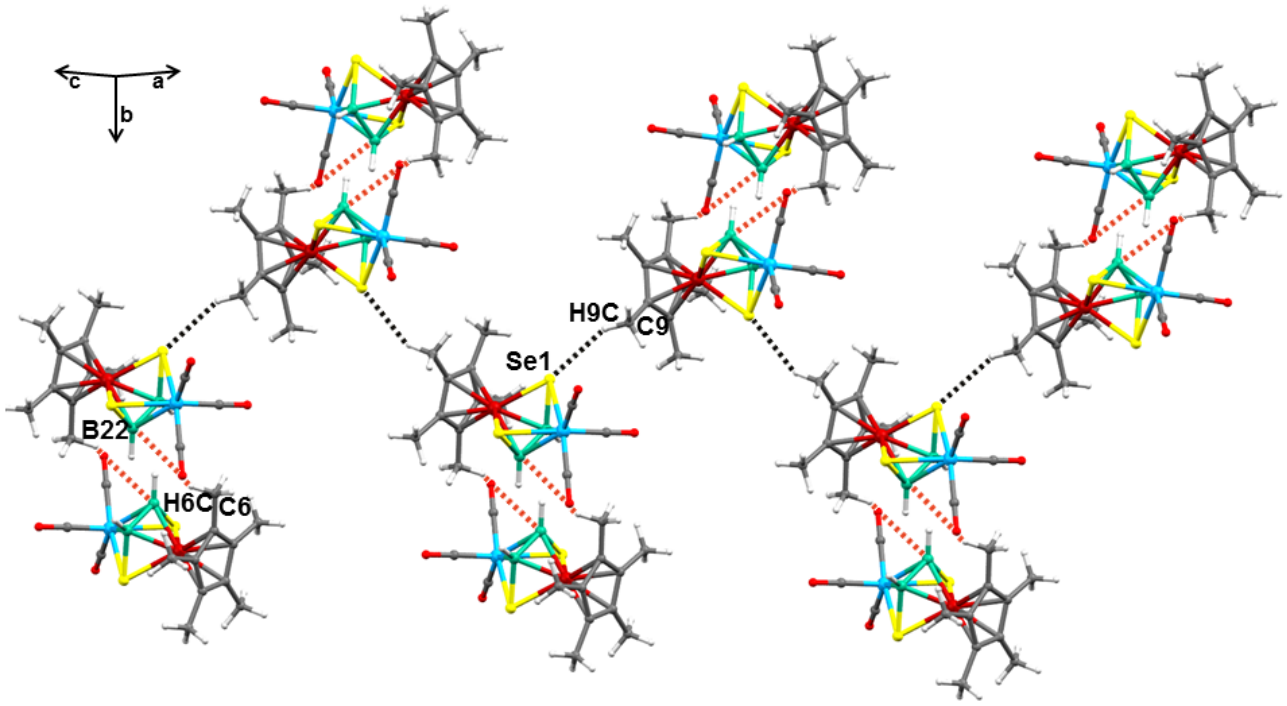

Fig. S4. 2D layer generated by intermolecular C-H...Se and weak C-H...B interactions in **2**.

Color code: Fe: cyan; C: dark gray; Co: scarlet; B: green; O: red and H: white.

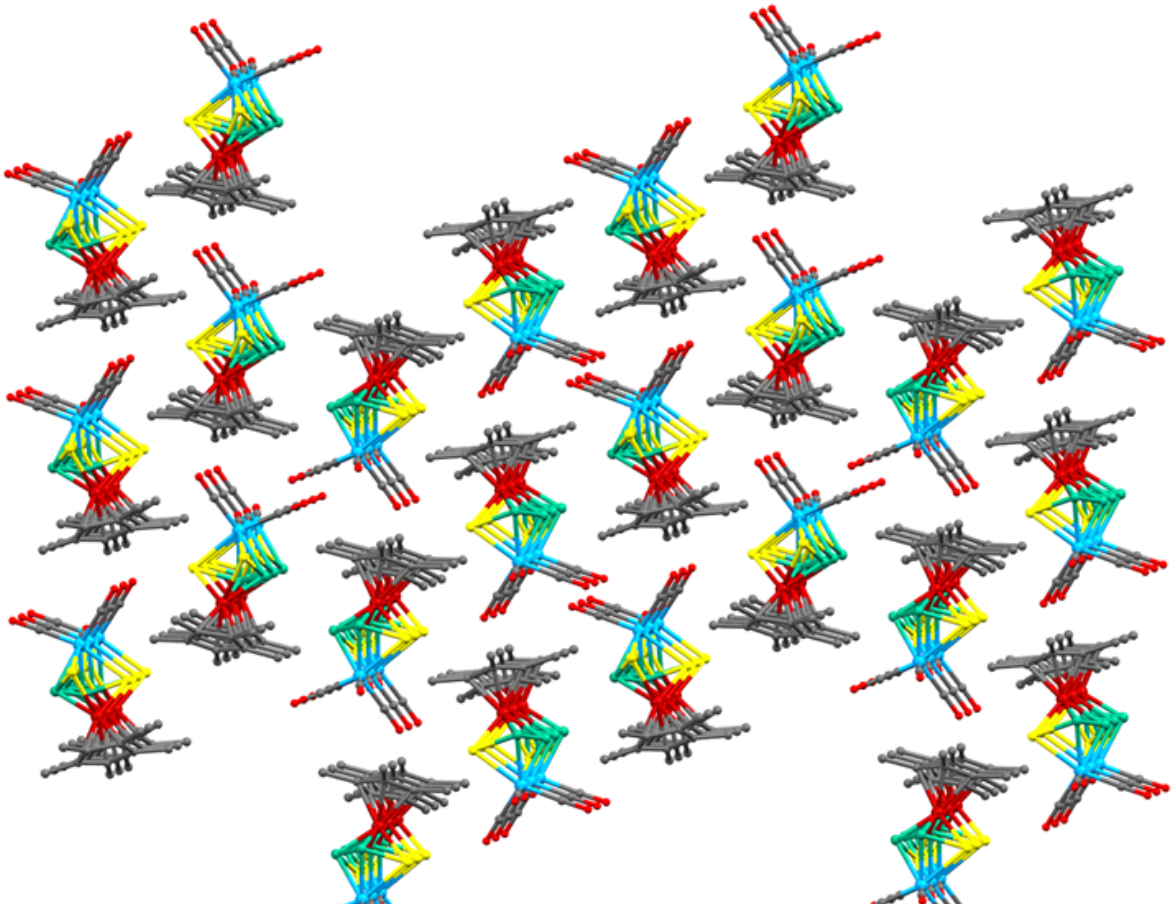

Fig. S5. Illustration of 3D arctitecture in **2** along *a* axis. Color code: Fe: cyan; C: dark gray; Co: scarlet; B: green; O: red (hydrogen atoms are removed for clarity).

Table S1. DFT calculated and experimental ^{11}B NMR and ^{1}H chemical shifts δ (ppm) values of compound **1** and **2**.

		1			**2**	
^{11}B NMR	Atom	Expt.	Calcd.	Atom	Expt.	Calcd.
	B1	33.5	31.85	B21	31.2	26.44
	B2	33.5	31.84	B22	31.2	26.44
^{1}H NMR	H1	3.67	5.53	H21	3.92	5.81
	H2	3.76	5.53	H22	3.85	5.81

The numbering of boron atoms and respective hyrogen atoms are given according to Fig. 1 and Fig. 5.