

SUPPLEMENTARY INFORMATION

**Chemistry of Group 9 Dimetallaborane Analogues of
Octaborane(12)**

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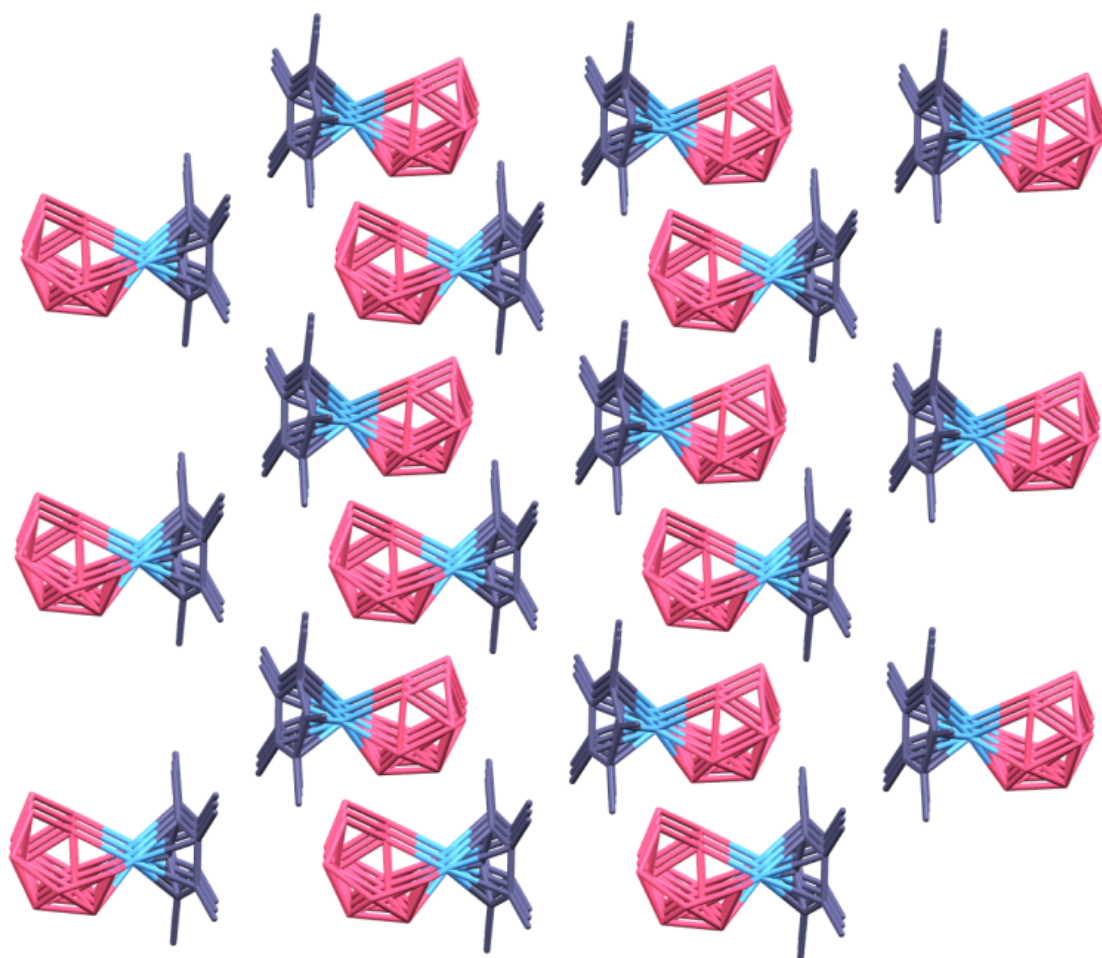


Fig. S1. Illustration of 3D packing view of **1** along *c* axis; Color code: C: violet; Co: cyan; B: pink; (hydrogen atoms are removed for clarity.)

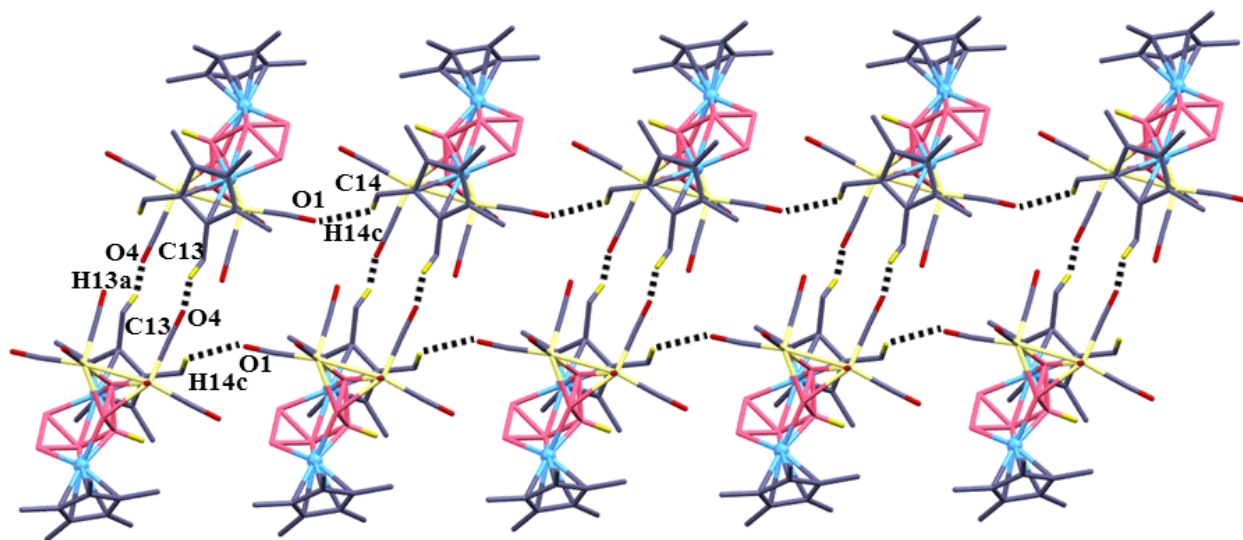


Fig. S2. The C-H...O hydrogen bonding interactions between the adjacent layered molecular units of **4** forming a 2D layer along the *c*-axis (hydrogen atoms except those, which have been taken part in the hydrogen bonding, are removed for clarity)

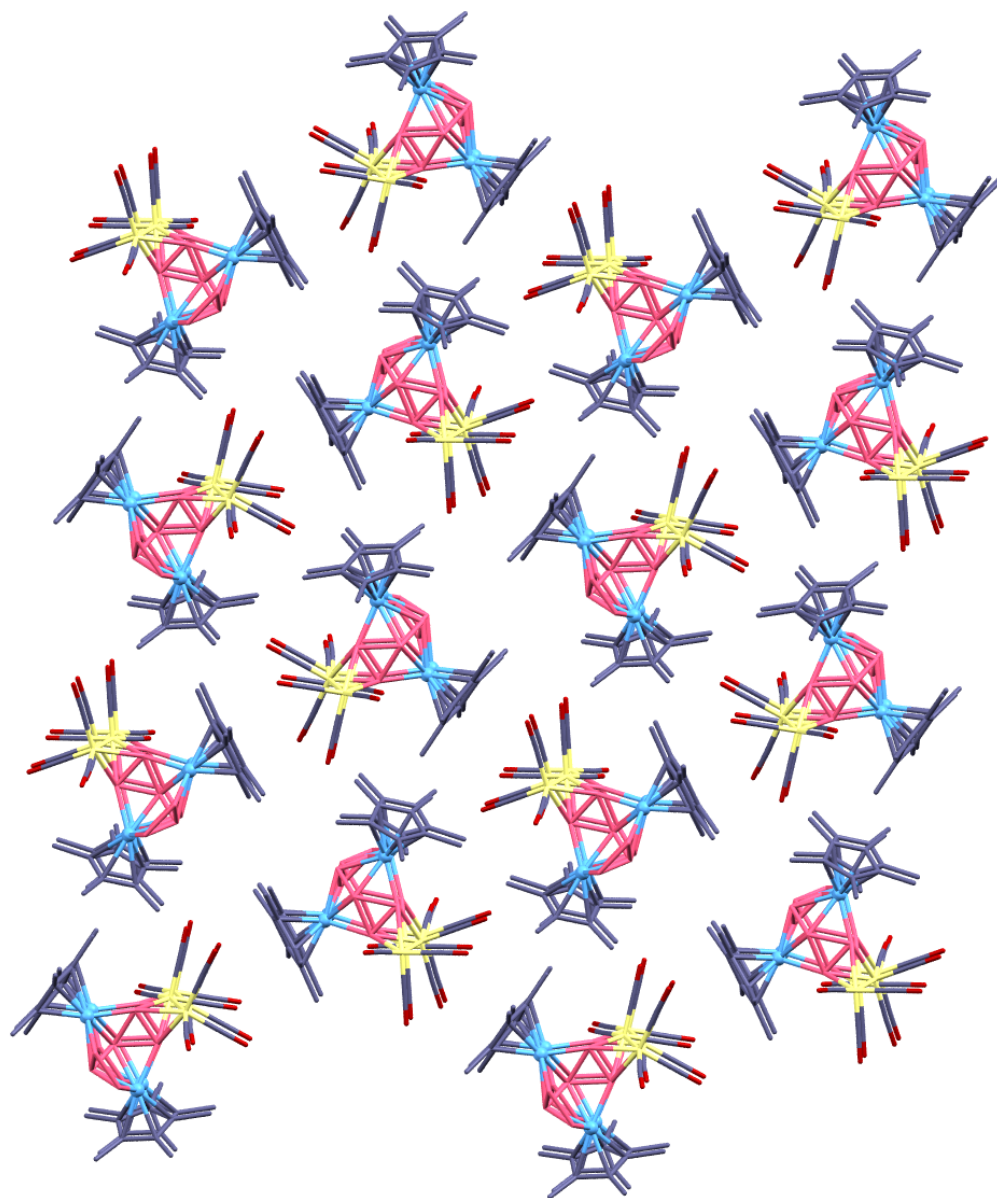


Fig. S3. 3D packing view along *a*-axis for **4** (hydrogen atoms are removed for clarity); Color code: Fe: Yellow; C: Violet; Co: Cyan; O: Scarlet red.

Table S1. Selected Structural Parameters and ^{11}B NMR Chemical Shifts of **4**,
 $[\{\text{Fe}_2(\text{CO})_6\}(\text{Cp}^*\text{Ru})_2(\text{CO})(\text{B}_6\text{H}_{10})]$ and $[\{\text{Fe}_2(\text{CO})_6\}(\text{Cp}^*\text{Rh})_2(\text{B}_6\text{H}_{10})]$

Compound	$\{\text{Fe}_2(\text{CO})_6\}(\text{Cp}^*\text{Ru})_2(\text{CO})(\text{B}_6\text{H}_{10})]$	$[\{\text{Fe}_2(\text{CO})_6\}(\text{Cp}^*\text{Rh})_2(\text{B}_6\text{H}_{10})]$	4
av $d_{\text{M-B}}$ (Å)	2.320	2.191	2.146
av $d_{\text{B-B}}$ (Å)	1.753	1.750	1.752
$d_{\text{Fe-Fe}}$ (Å)	2.569	2.580	2.578
av $d_{\text{B-B}}$ (Å)	1.711	1.706	1.687
$d_{\text{B-B}}$ (Å) ^a	1.711	1.701	1.687
Dihedral angle (deg) ^b	149.77	151.69	152.00
^{11}B NMR	47.1, 37.1, 29.9, 1.37, -2.70	34.7, 28.1, 25.2, 16.4, 1.6, -12.3	45.5, 32.02, 26.94, 25.30, 9.08, -5.50

a distance between the fused B-B bond between two polyhedral, *b* angle between the planes

shown in the Chart 1