

Supporting Information

$\text{B}_{12}(\text{SCN})_{12}^{2-}$: An Ultra-Stable Weakly-Coordinating Dianion

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Table S1 Optimized bond lengths of the dianion, monoanion and neutral states of $\text{B}_{12}(\text{SCN})_{12}$, $\text{CB}_{11}(\text{SCN})_{12}$ and $\text{B}_{12}(\text{OCN})_{12}$. For $\text{CB}_{11}(\text{SCN})_{12}$, C_1 is the carbon that constitutes the cage and C_2 is the carbon in the $\text{C}_1\text{N}_\text{C}\text{C}_2\text{S}_\text{C}$ branch.

Bond	Dianion (Å)	Monoanion (Å)	Neutral (Å)
$\text{B}_{12}(\text{SCN})_{12}$			
B-B	1.80	1.81	1.82
B-N	1.44	1.43	1.42
N-C	1.19	1.19	1.19
C-S	1.60	1.59	1.58
$\text{CB}_{11}(\text{SCN})_{12}$			
B-B	--	1.81	1.82
B-N	--	1.42	1.41
N-C	--	1.19	1.20
C-S	--	1.59	1.58
$\text{C}_1\text{-B}$	--	1.75	1.76
$\text{C}_1\text{-N}_\text{C}$	--	1.38	1.38
$\text{N}_\text{C}\text{-C}_2$	--	1.20	1.21
$\text{C}_2\text{-S}_\text{C}$	--	1.57	1.57
$\text{B}_{12}(\text{OCN})_{12}$			
B-B	1.80	1.81	1.83
B-N	1.45	1.43	1.42
N-C	1.19	1.19	1.20
C-O	1.19	1.18	1.18

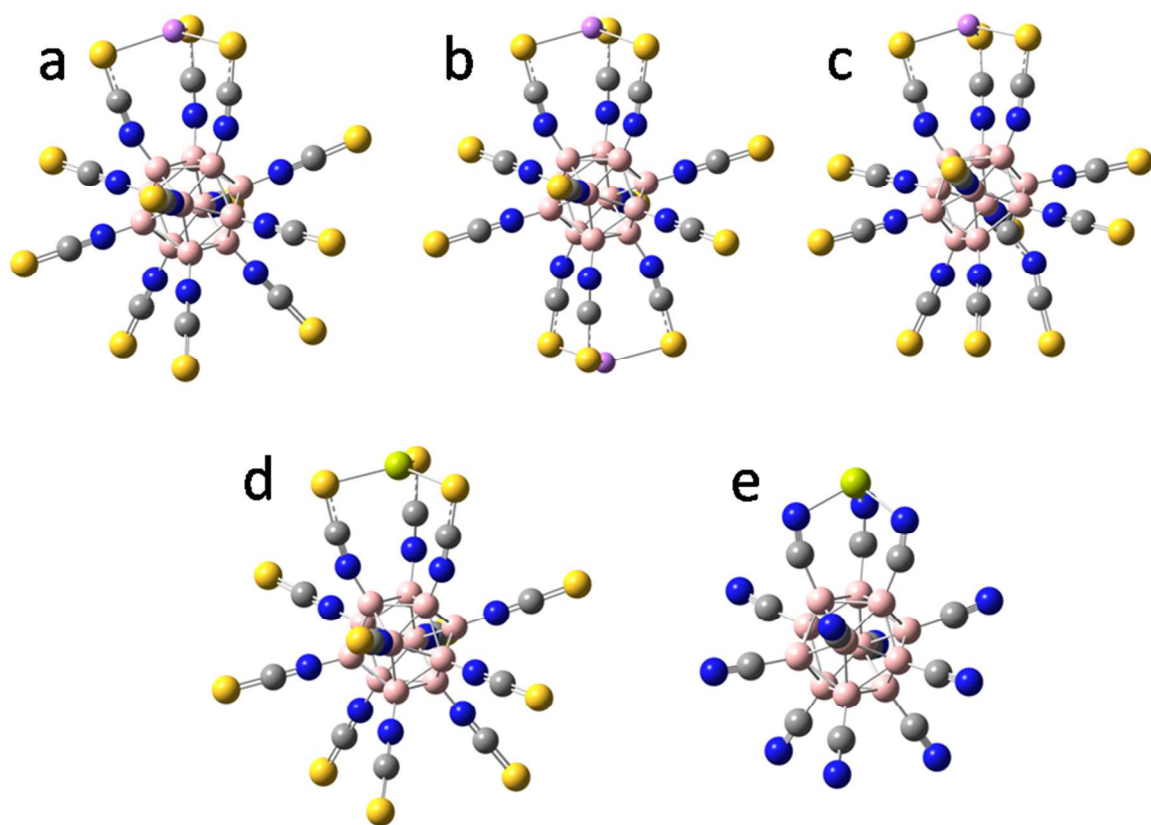


Fig. S1 Ground states of (a) $[\text{LiB}_{12}(\text{SCN})_{12}]^{-}$, (b) $\text{Li}_2\text{B}_{12}(\text{SCN})_{12}$, (c) $\text{LiCB}_{11}(\text{SCN})_{12}$, (d) $\text{MgB}_{12}(\text{SCN})_{12}$ and (e) $\text{MgB}_{12}(\text{CN})_{12}$. Li is in magenta, S is in yellow, C is in grey, N is in blue, B is in pink, and Mg is in green-yellow.

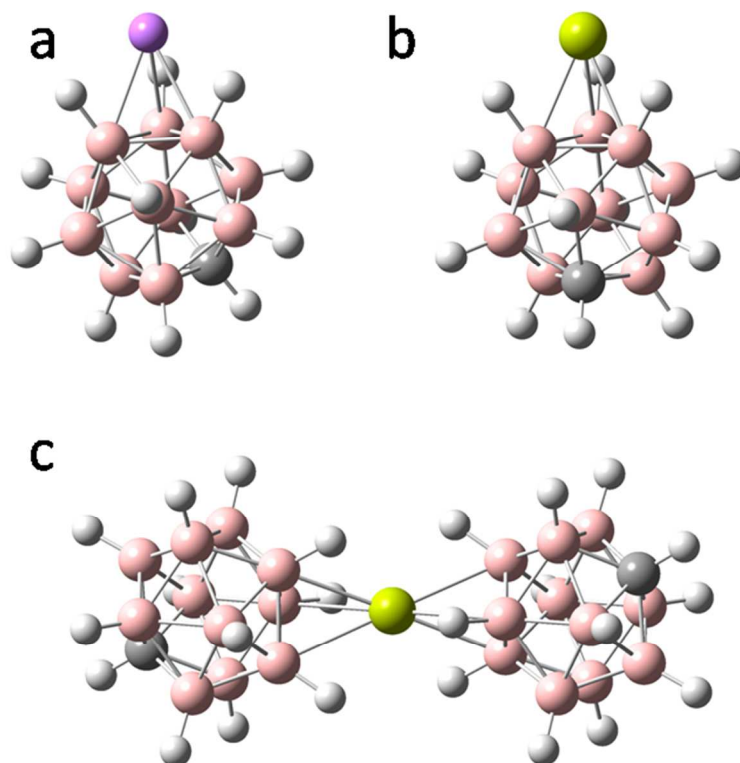


Fig. S2 Ground states of (a) $\text{LiCB}_{11}\text{H}_{12}$, (b) $[\text{MgCB}_{11}\text{H}_{12}]^+$ and (c) $\text{Mg}(\text{CB}_{11}\text{H}_{12})_2$. Li is in magenta, H is in white, B is in pink, C is in grey, N is in blue and Mg is in green-yellow.