On the Electronic Structure and Stability of Icosahedral *r*-$X_2Z_{10}H_{12}$ and $Z_{12}H_{12}^{2-}$ Clusters; *r* = {*ortho*, *meta*, *para*}, X = {C, Si} , Z = {B, Al}*

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SUPPLEMENTARY INFORMATION: This section includes the experimental (where available) and computed symmetry-unique cage distances, Mulliken and natural bond orbital (NBO) charges [1], as well as the atom-in-molecules (AIM) topological analysis of the electron density for the $Z_{12}H_{12}^{2-}$ and *r*-$X_2Z_{10}H_{12}$ clusters; X = {C, Si}, Z = {B, Al}, *r* = {*ortho*, *meta*, *para*}. All computations carried out with the B3LYP/6-311+G(d,p) model. We also include the continuous shape measures S_{IC} [2] for the available crystal structures of the clusters included in this work (Table S3). In the colour PDF or HTML file, bond critical points, ring critical points and cage critical points - Figure S1, from (a) to (n) - are represented in small red, yellow and green spheres respectively.

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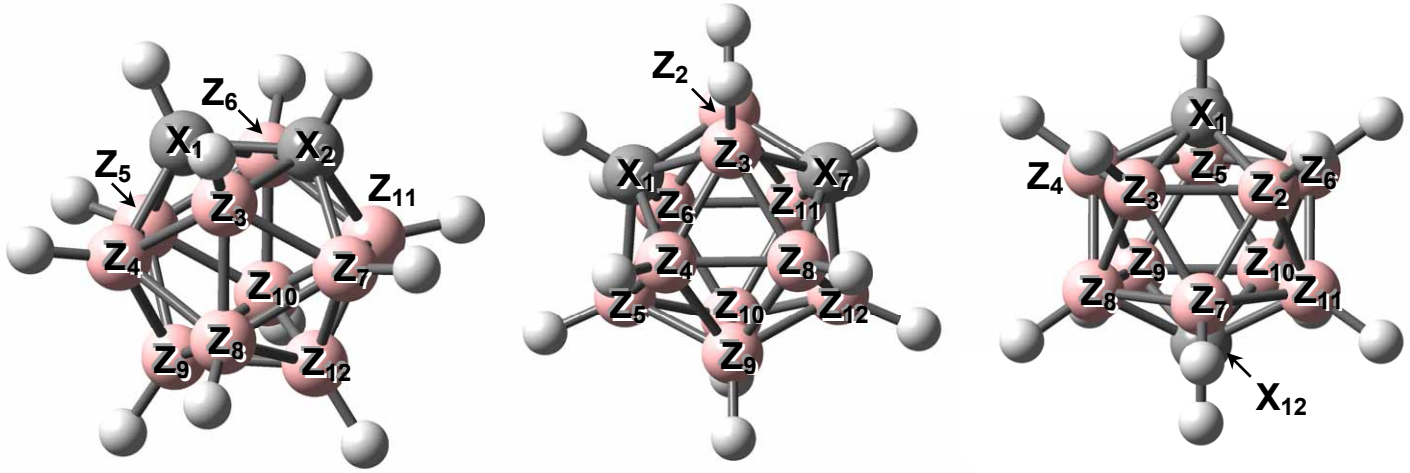


Table S1. Experimental (where available) and computed symmetry-unique cage distances for $Z_{12}H_{12}^{2-}$ and *r*-$X_2Z_{10}H_{12}$ clusters; X = {C, Si}, Z = {B, Al}, *r* = {*ortho*, *meta*, *para*}. All computations with the B3LYP/6-311+G(d,p) model. Distance = Computed/*Experimental*. Relative error: $|\varepsilon_\Delta| = |(d_{comp} - d_{exp})/d_{exp}| \times 100$ (%).

↓Z/→X	X=Z	Comp/*Exp*	$\|\varepsilon_\Delta\|$							
Z=B	Z_1Z_2	1.786/*1.785* [3]	0.1							
Z=Al	Z_1Z_2	2.702/*2.702* [4]	0.0		Comp/*Exp*					
				Comp	R=Me		↓Z\→X			
	Ortho	X=C [5]		X=Si	X=Si [6]	$\|\varepsilon_\Delta\|$		Ortho	X=C	X=Si
Z=B	X_1X_2	1.625/*1.626*	0.4	2.314	2.325/*2.308*	0.7	Z=Al	X_1X_2	1.632	2.448
	X_1Z_3	1.720/*1.717*	0.2	2.139	2.138/*2.117*	1.0		X_1Z_3	2.158	2.620
	X_1Z_4	1.698/*1.689*	0.5	2.025	2.026/*2.018*	0.4		X_1Z_4	2.253	2.572
	Z_3Z_4	1.779/*1.765*	0.8	1.862	1.854/*1.848*	0.3		Z_3Z_4	2.566	2.714
	Z_3Z_8	1.764/*1.760*	0.2	1.777	1.779/*1.770*	0.5		Z_3Z_8	2.678	2.657
	Z_4Z_5	1.785/*1.785*	0.0	1.890	1.881/*1.859*	1.2		Z_4Z_5	2.579	2.752
	Z_4Z_8	1.781/*1.773*	0.5	1.775	1.773/*1.774*	0.1		Z_4Z_8	2.651	2.697
	Z_4Z_9	1.777/*1.768*	0.5	1.775	1.774/*1.765*	0.5		Z_4Z_9	2.650	2.680
	Z_8Z_9	1.793/*1.789*	0.2	1.789	1.788/*1.783*	0.3		Z_8Z_9	2.785	2.728
	Z_9Z_{12}	1.783/*1.780*	0.2	1.779	1.778/*1.774*	0.2		Z_9Z_{12}	2.711	2.699
Z=B	Meta	X=C [7]	$\|\varepsilon_\Delta\|$	X=Si			Z=Al	Meta	X=C	X=Si
	X_1Z_2	1.693/*1.693*	0.0	2.033				X_1Z_2	2.176	2.562
	X_1Z_4	1.714/*1.709*	0.3	2.045				X_1Z_4	2.358	2.617
	X_1Z_5	1.711/*1.708*	0.2	2.032				X_1Z_5	2.207	2.586
	Z_2Z_3	1.789/*1.778*	0.6	2.036				Z_2Z_3	2.453	2.788
	Z_3Z_4	1.767/*1.763*	0.2	1.848				Z_3Z_4	2.515	2.688
	Z_4Z_5	1.783/*1.777*	0.3	1.872				Z_4Z_5	2.561	2.728
	Z_4Z_8	1.771/*1.767*	0.2	1.764				Z_4Z_8	2.651	2.664
	Z_4Z_9	1.780/*1.777*	0.2	1.784				Z_4Z_9	2.693	2.699
	Z_5Z_9	1.778/*1.772*	0.3	1.774				Z_5Z_9	2.678	2.682
	Z_9Z_{10}	1.793/*1.782*	0.6	1.798				Z_9Z_{10}	2.787	2.749
Z = B	Para	X=C [6]	$\|\varepsilon_\Delta\|$(%)	X=Si			Z=Al	Para	X=C	X=Si
	X_1Z_2	1.708/*1.712*	0.2	2.037				X_1Z_2	2.265	2.590
	Z_2Z_3	1.786/*1.785*	0.1	1.889				Z_2Z_3	2.575	2.755
	Z_2-Z_7	1.767/*1.772*	0.3	1.762				Z_2-Z_7	2.619	2.653

Table S2. Mulliken and NBO (Natural Bond Orbital) charges (in units of $|e|$) for the $Z_{12}H_{12}^{2-}$ and *r*-$X_2Z_{10}H_{12}$ clusters included in this work, *r* = {*ortho*, *meta*, *para*}, X = {C, Si}, Z = {B, Al}. Computations on the optimized geometries at B3LYP/6-311+G(d,p) level of theory. Note: The atom labels follow from Figure 1 in main text and Table S1 above. The hydrogen labels are equivalent to cage atom labels, namely, H(*j*) is bound to Z(*j*) or X(*j*).

Cluster	Atom	*q*(Mulliken)	*q*(NBO)				
$B_{12}H_{12}^{2-}$	B_1	-0.027	-0.175				
	H_1	-0.140	0.008				
$Al_{12}H_{12}^{2-}$	Al_1	0.033	0.117				
	H_1	-0.200	-0.283	Cluster	Atom	*q*(Mulliken)	*q*(NBO)
o-$C_2B_{10}H_{12}$	C_1	-0.146	-0.496	*o*-$Si_2B_{10}H_{12}$	Si_1	0.764	0.892
	H_1	0.247	0.300		H_1	0.024	-0.025
	B_3	-0.114	0.158		B_3	-0.655	-0.333
	H_3	0.019	0.054		H_3	0.061	0.058
	B_4	-0.158	0.000		B_4	-0.307	-0.286
	H_4	0.017	0.069		H_4	0.059	0.078
	B_8	0.127	-0.165		B_8	0.191	-0.185
	H_8	0.014	0.078		H_8	0.035	0.082
	B_9	0.122	-0.139		B_9	0.050	-0.153
	H_9	0.015	0.073		H_9	0.025	0.079
m-$C_2B_{10}H_{12}$	C_1	-0.052	-0.639	*m*-$Si_2B_{10}H_{12}$	Si_1	1.160	1.083
	H_1	0.233	0.299		H_1	0.020	-0.028
	B_3	-0.367	0.149		B_3	-0.720	-0.436
	H_3	0.037	0.066		H_3	0.070	0.074
	B_4	0.015	-0.021		B_4	-0.242	-0.280
	H_4	0.018	0.073		H_4	0.054	0.076
	B_5	-0.115	0.058		B_5	-0.414	-0.267
	H_5	0.016	0.056		H_5	0.045	0.074
	B_9	0.170	-0.176		B_9	0.182	-0.173
	H_9	0.014	0.080		H_9	0.035	0.079
p-$C_2B_{10}H_{12}$	C_1	-0.157	-0.664	*p*-$Si_2B_{10}H_{12}$	Si_1	0.995	1.094
	H_1	0.242	0.299		H_1	0.021	-0.028
	B_2	-0.038	0.005		B_2	-0.256	-0.289
	H_2	0.021	0.068		H_2	0.053	0.076

Table S2 (cont)

Cluster	Atom	*q*(Mulliken)	*q*(NBO)	Cluster	Atom	*q*(Mulliken)	*q*(NBO)
o-$C_2Al_{10}H_{12}$	C_1	-0.313	-1.239	*o*-$Si_2Al_{10}H_{12}$	Si_1	-0.011	-0.196
	H_1	0.234	0.276		H_1	0.012	-0.025
	Al_3	0.292	0.805		Al_3	0.108	0.392
	H_3	-0.137	-0.255		H_3	-0.103	-0.231
	Al_4	0.037	0.442		Al_4	0.031	0.294
	H_4	-0.125	-0.230		H_4	-0.102	-0.229
	Al_8	0.239	0.240		Al_8	0.136	0.186
	H_8	-0.115	-0.246		H_8	-0.101	-0.229
	Al_9	0.092	0.239		Al_9	0.204	0.201
	H_9	-0.117	-0.244		H_9	-0.104	-0.229
m-$C_2Al_{10}H_{12}$	C_1	-0.395	-1.623	*m*-$Si_2Al_{10}H_{12}$	Si_1	-0.028	-0.320
	H_1	0.210	0.267		H_1	0.004	-0.030
	Al_3	0.254	0.819		Al_3	0.118	0.408
	H_3	-0.125	-0.231		H_3	-0.104	-0.226
	Al_4	0.126	0.503		Al_4	0.084	0.296
	H_4	-0.125	-0.238		H_4	-0.103	-0.228
	Al_5	0.242	0.505		Al_5	0.169	0.313
	H_5	-0.125	-0.231		H_5	-0.106	-0.229
	Al_9	0.058	0.208		Al_9	0.086	0.176
	H_9	-0.119	-0.243		H_9	-0.101	-0.227
p-$C_2Al_{10}H_{12}$	C_1	-0.285	-1.604	*p*-$Si_2Al_{10}H_{12}$	Si_1	0.027	-0.324
	H_1	0.210	0.271		H_1	-0.001	-0.031
	Al_2	0.143	0.500		Al_2	0.098	0.299
	H_2	-0.128	-0.233		H_2	-0.103	-0.228

Table S3. Continuous shape measures (S_{IC}) [2] for experimental available crystal structures of borane ($B_{12}R_{12}^{2-}$), *o*-carborane, *m*-carborane, *p*-carborane, *o*-silaborane and alane $Al_{12}R_{12}^{2-}$.

BORANES

Reference*	Experimental values (Å) Mean B-B distance	S_{IC}
[8]	1.779	0.015
[8]	1.775	0.022
[9]	1.786	0.001
[10]	1.776	0.008
[11]	1.776	0.052
[12]	1.783	0.013
[12]	1.775	0.028
[13]	1.793	0.002
[14]	1.790	0.003
[14]	1.782	0.003
[15]	1.783	0.002
[16]	1.784	0.001
$(K^+)_2\,[B_{12}H_{12}]^{2-}$ [3]	1.779	0.001
$(Rb^+)_2\,[B_{12}H_{12}]^{2-}$ [3]	1.782	0.001
[17]	1.817	0.019
[18]	1.777	0.001
$(K^+)_3\,[B_{12}H_{12}]^{2-}\,I^-$ [3]	1.774	0.002
$(K^+)_3\,[B_{12}H_{12}]^{2-}\,I^-$ [3]	1.781	0.001
$(Cs^+)_3\,[B_{12}H_{12}]^{2-}\,I^-$ [3]	1.783	0.001
$(Rb^+)_3\,[B_{12}H_{12}]^{2-}\,Cl^-$ [18]	1.776	0.000
$(Rb^+)_3\,[B_{12}H_{12}]^{2-}\,Br^-$ [18]	1.778	0.000
$(Cs^+)_3\,[B_{12}H_{12}]^{2-}\,Br^-$ [18]	1.782	0.001
$(Cs^+)_3\,[B_{12}H_{12}]^{2-}\,Cl^-$ [18]	1.782	0.000
[19]	1.787	0.004
[19]	1.770	0.006
[20]	1.782	0.024
$(NH_4^+)_2\,[B_{12}H_{12}]^{2-}$ [3]	1.785	0.000
$(NH_4^+)_3\,[B_{12}H_{12}]^{2-}\,I^-$ [3]	1.781	0.000
[21]	1.776	0.001
$(NH_4^+)_3\,[B_{12}H_{12}]^{2-}\,Br^-$ [18]	1.782	0.000
[22]	1.775	0.002
[23]	1.763	0.008
[24]	1.785	0.007
[24]	1.785	0.031
[25]	1.782	0.001
[26]	1.776	0.004
[27]	1.773	0.005
[28]	1.792	0.002

* Same reference for different row refers to a different crystal/counterion(s) (cations and anions other than $B_{12}H_{12}^{2-}$). The ions are indicated in certain cases for clarity.

Table S3 (cont)

***ORTHO*-CARBORANE**

	Experimental distances (Å)										S_{IC}
Reference*	C-C	C-B_A	C-B_B	B_A-B_B	B_A-B_C	B_B-B_B	B_B-B_C	B_B-B_D	B_C-B_D	B_D-B_D	
[29]	1.647	1.679	1.711	1.743	1.726	1.765	1.776	1.773	1.781	1.756	0.110
[5]	1.645	1.717	1.703	1.771	1.760	1.778	1.778	1.774	1.785	1.785	0.081
[5]	1.626	1.717	1.689	1.765	1.760	1.785	1.773	1.768	1.789	1.780	0.126
[30]	1.633	1.723	1.711	1.764	1.763	1.782	1.778	1.776	1.788	1.796	0.087
[30]	1.637	1.700	1.701	1.767	1.744	1.782	1.767	1.765	1.774	1.792	0.086
[30]	1.620	1.712	1.686	1.765	1.757	1.775	1.774	1.773	1.786	1.775	0.117
[31]	1.595	1.667	1.680	1.710	1.707	1.740	1.742	1.730	1.752	1.762	0.103
[32]	1.626	1.706	1.692	1.796	1.782	1.767	1.781	1.781	1.775	1.777	0.101
[33]	1.627	1.704	1.684	1.760	1.752	1.773	1.772	1.663	1.770	1.755	0.113
[33]	1.599	1.693	1.671	1.762	1.761	1.778	1.753	1.751	1.762	1.777	0.142
[33]	1.610	1.675	1.643	1.699	1.759	1.803	1.742	1.718	1.779	1.869	0.245
[34]	1.708	1.712	1.694	1.719	1.760	1.796	1.699	1.717	1.790	1.910	0.114
[34]	1.584	1.704	1.645	1.660	1.668	1.724	1.774	1.768	1.737	1.788	0.195
[34]	1.706	1.705	1.703	1.729	1.755	1.774	1.712	1.717	1.763	1.806	0.051
[35]	1.429	1.658	1.804	1.727	1.651	1.750	1.704	1.776	1.721	1.474	0.304
[36]	1.666	1.700	1.685	1.753	1.723	1.783	1.752	1.760	1.764	1.762	0.080
[37]	1.624	1.713	1.693	1.768	1.769	1.777	1.771	1.768	1.784	1.776	0.107
[37]	1.625	1.704	1.690	1.758	1.763	1.775	1.773	1.774	1.778	1.764	0.101
[38]	1.622	1.694	1.691	1.745	1.743	1.752	1.757	1.738	1.762	1.763	0.110
[39]	1.683	1.719	1.713	1.767	1.770	1.711	1.746	1.742	1.765	1.778	0.070

* Same reference for a different row refers to a different crystal/counterion(s) (see reference).

***META*-CARBORANE**

	Experimental distances (Å)											S_{IC}
Ref*	C···C	B_A-B_A	B_B-B_B	B_D-B_D	C-B_A	C-B_B	C-B_C	B_A-B_B	B_B-B_C	B_B-B_D	B_C-B_D	
[7]	2.614	1.778	1.767	1.782	1.693	1.709	1.708	1.763	1.777	1.777	1.772	0.101
[34]	2.715	1.674	1.706	1.737	1.683	1.671	1.706	1.684	1.720	1.727	1.724	0.062
[34]	2.748	1.693	1.707	1.747	1.696	1.704	1.747	1.702	1.743	1.731	1.740	0.055
[34]	2.601	1.779	1.768	1.785	1.687	1.707	1.710	1.761	1.777	1.772	1.770	0.109
[34]	2.695	1.656	1.685	1.735	1.672	1.676	1.723	1.689	1.637	1.728	1.720	0.068
[34]	2.666	1.769	1.731	1.767	1.695	1.715	1.735	1.735	1.755	1.757	1.750	0.050
[37]	2.609	1.774	1.762	1.768	1.693	1.705	1.708	1.771	1.767	1.771	1.756	0.103

* Same reference for a different row refers to a different crystal/counterion(s) (see reference).

***PARA*-CARBORANE**

	Experimental distances (Å)				S_{IC}
Reference*	C···C	B-B	C-B	B-B$^{\$}$	
[7]	3.071	1.777	1.704	1.765	0.117
[7]	3.083	1.785	1.712	1.772	0.118
[37]	3.052	1.781	1.704	1.762	0.137
[37]	3.060	1.781	1.706	1.760	0.131

* Same reference for a different row refers to a different crystal/counterion(s) (see reference).
B-B: same pentagon
B-B$^{\$}$: between pentagons

ORTHO-SILABORANE

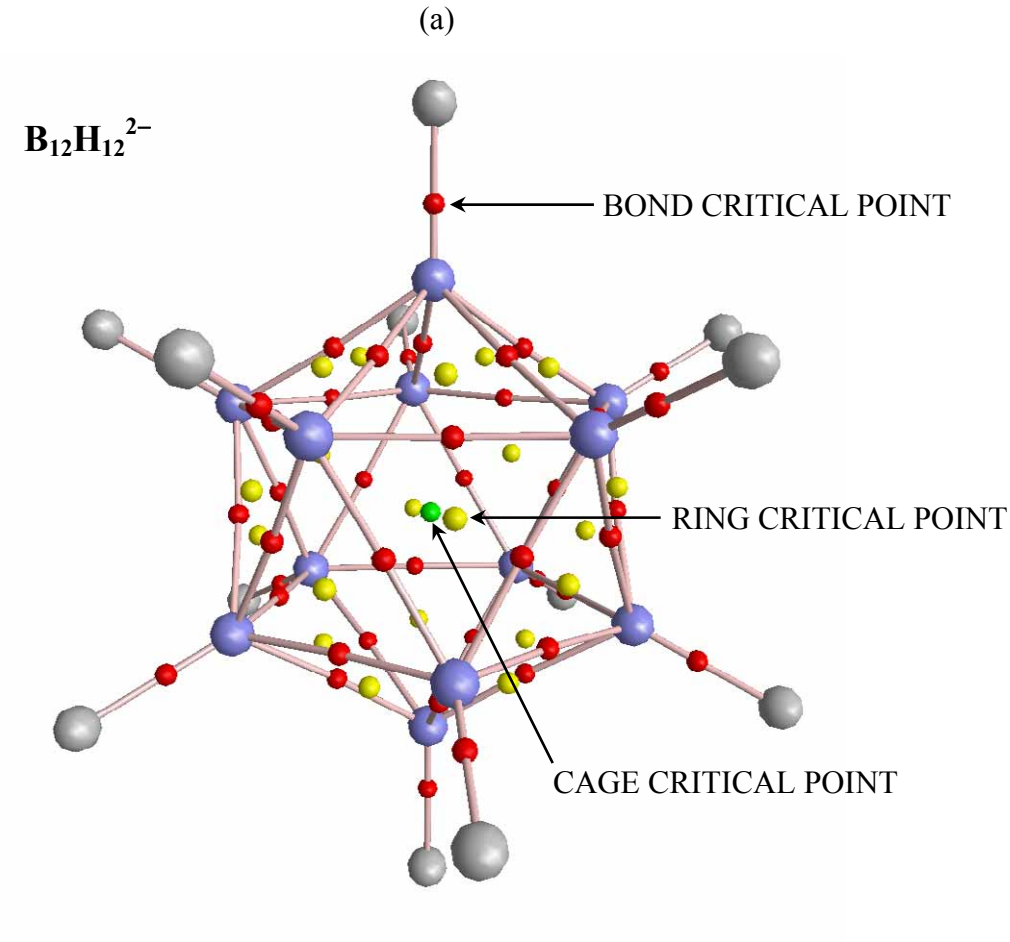
	Experimental distances (Å)										S_{IC}
Reference	Si-Si	Si-B_A	Si-B_B	B_A-B_B	B_A-B_C	B_B-B_B	B_B-B_C	B_B-B_D	B_C-B_D	B_D-B_D	
[40]	2.314	2.111	2.014	1.854	1.780	1.863	1.771	1.766	1.782	1.780	0.575
[41]	2.304	2.110	2.021	1.844	1.780	1.864	1.759	1.764	1.775	1.750	0.605
[6]	2.308	2.115	2.017	1.849	1.770	1.859	1.770	1.767	1.782	1.774	0.585
[42]	2.308	2.115	2.017	1.849	1.770	1.859	1.770	1.767	1.782	1.774	0.585

ALANES

	Experimental values (Å)	S_{IC}
Reference*	Mean Al-Al distance	
[43]	2.686	0.001
[4]	2.701	0.157
[4]	2.702	0.146
[44]	2.684	0.019
[44]	2.685	0.024

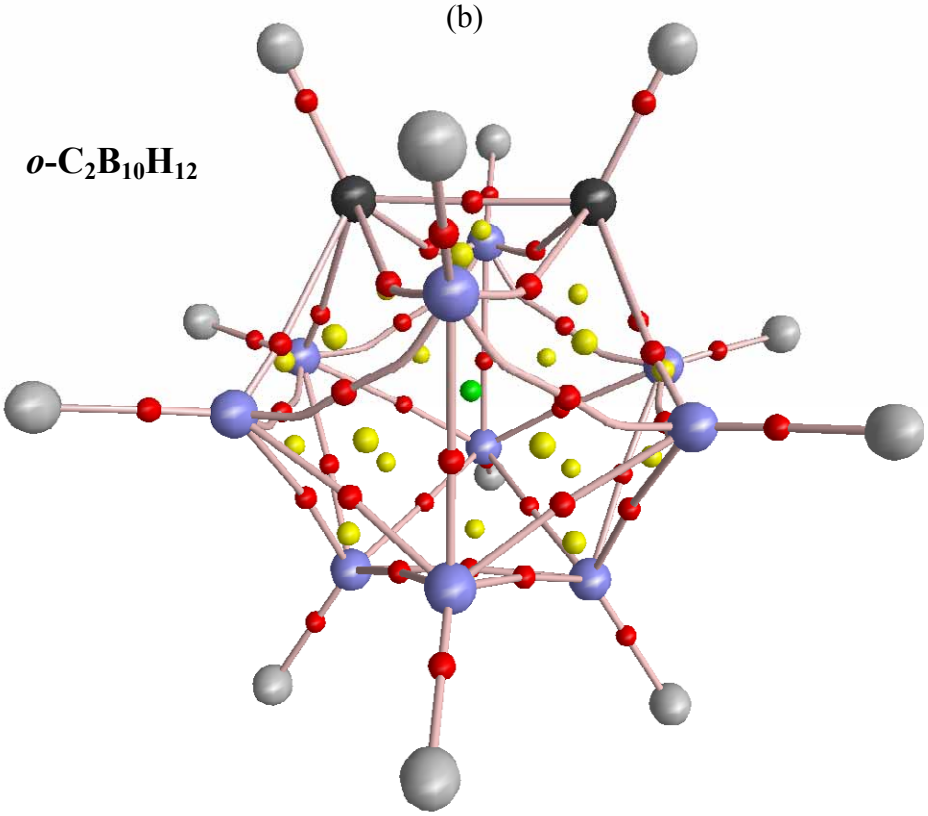
* Same reference for a different row refers to a different crystal/counterion(s) (see reference).

Figure S1. Topological analysis of the electron density in $Z_{12}H_{12}^{2-}$ and *r*-$X_2Z_{10}H_{12}$ clusters with X = {C, Si} and Z={B, Al}. (a) $B_{12}H_{12}^{2-}$, (b) *ortho*-$C_2B_{10}H_{12}$, (c) *meta*-$C_2B_{10}H_{12}$, (d) *para*-$C_2B_{10}H_{12}$, (e) *ortho*-$Si_2B_{10}H_{12}$, (f) *meta*-$Si_2B_{10}H_{12}$, (g) *para*-$Si_2B_{10}H_{12}$, (h) $Al_{12}H_{12}^{2-}$, (i) *ortho*-$C_2Al_{10}H_{12}$, (j) *meta*-$C_2Al_{10}H_{12}$, (k) *para*-$C_2Al_{10}H_{12}$, (l) *ortho*-$Si_2Al_{10}H_{12}$, (m) *meta*-$Si_2Al_{10}H_{12}$, (n) *para*-$Si_2Al_{10}H_{12}$. Computations with the B3LYP/6-311+G(d,p) model. All geometries correspond to energy minima.



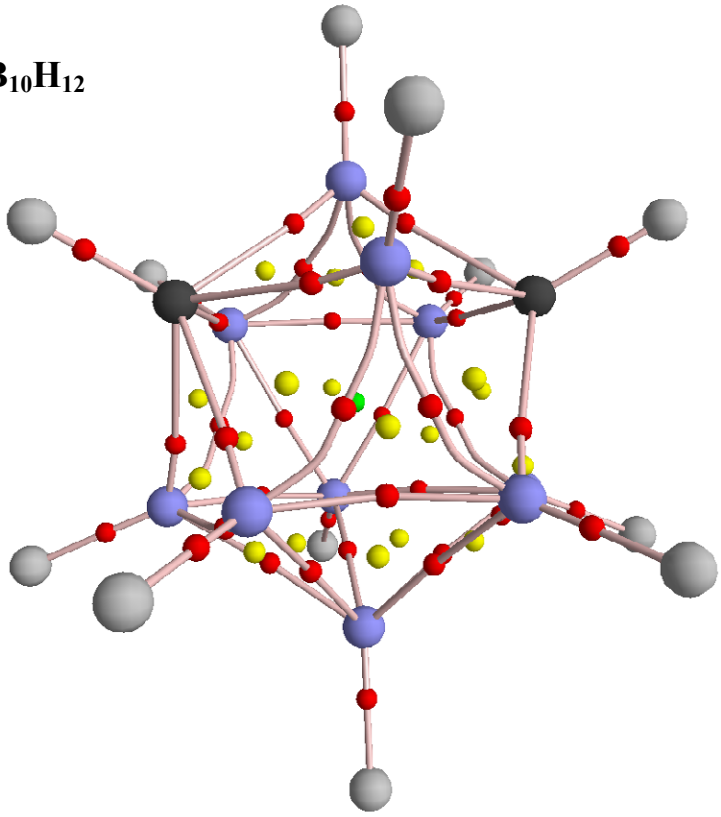
(b)

***o*-$C_2B_{10}H_{12}$**



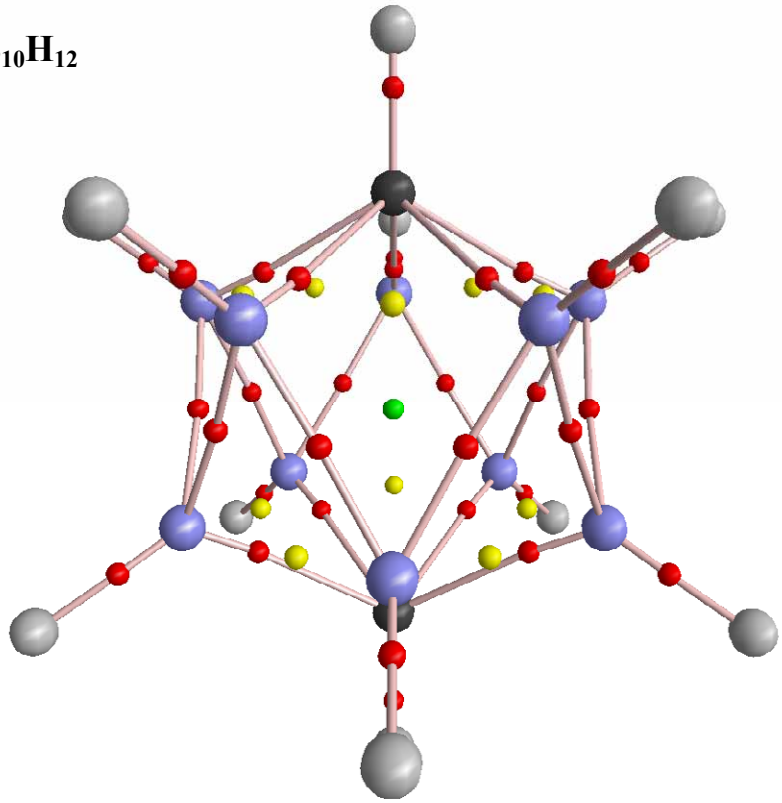
(c)

***m*-$C_2B_{10}H_{12}$**



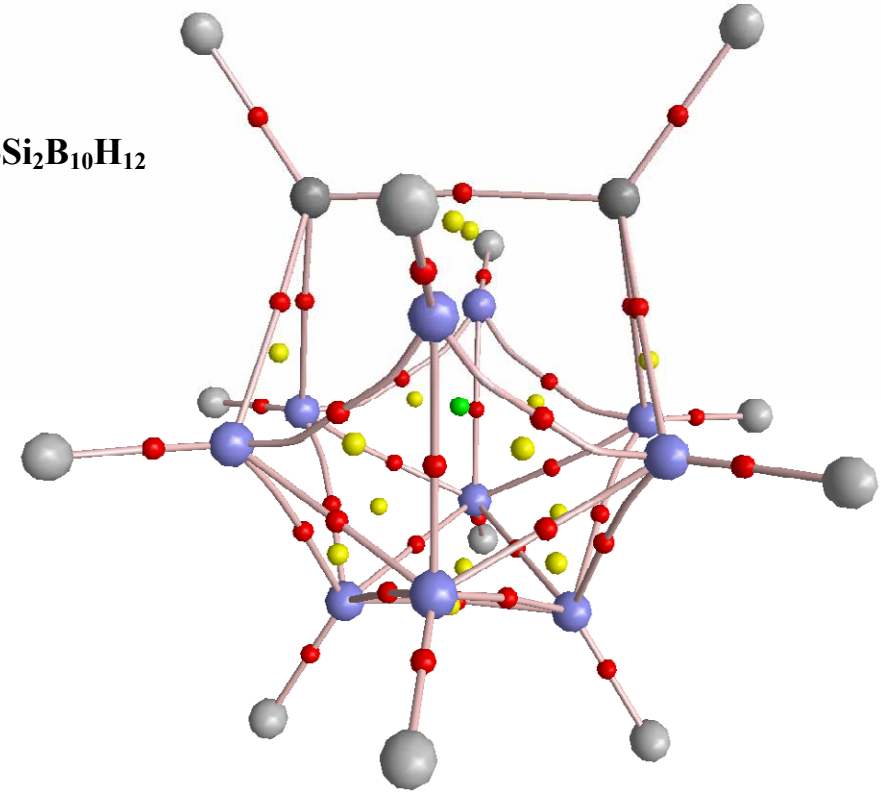
(d)

***p*-$C_2B_{10}H_{12}$**

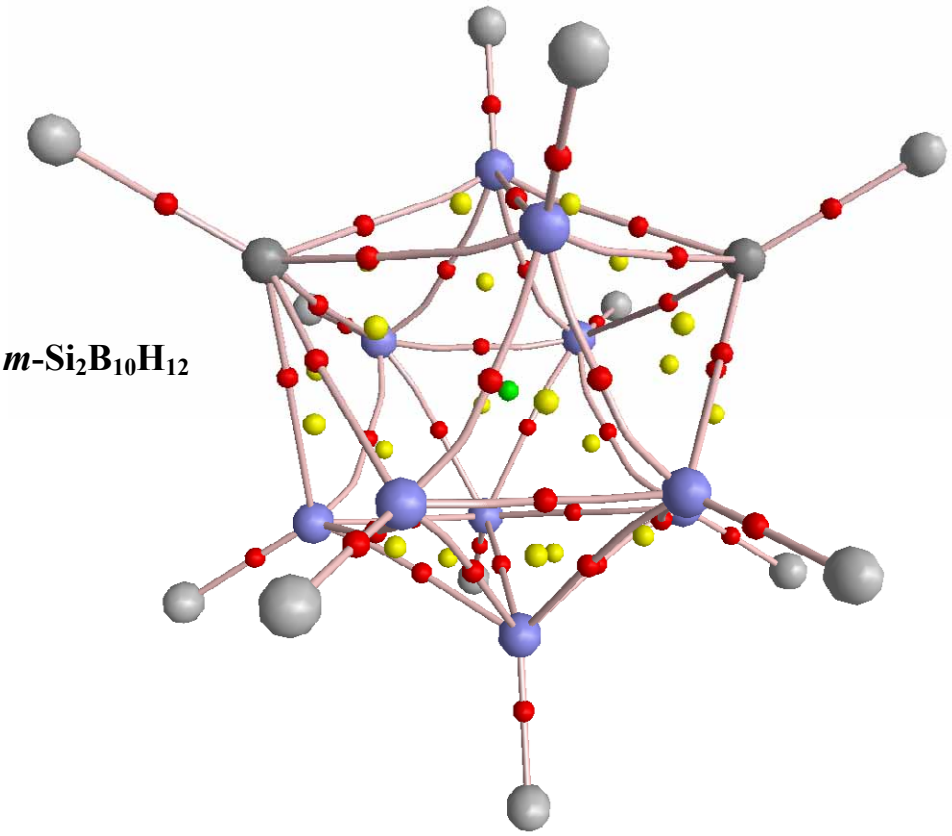


(e)

***o*-$Si_2B_{10}H_{12}$**

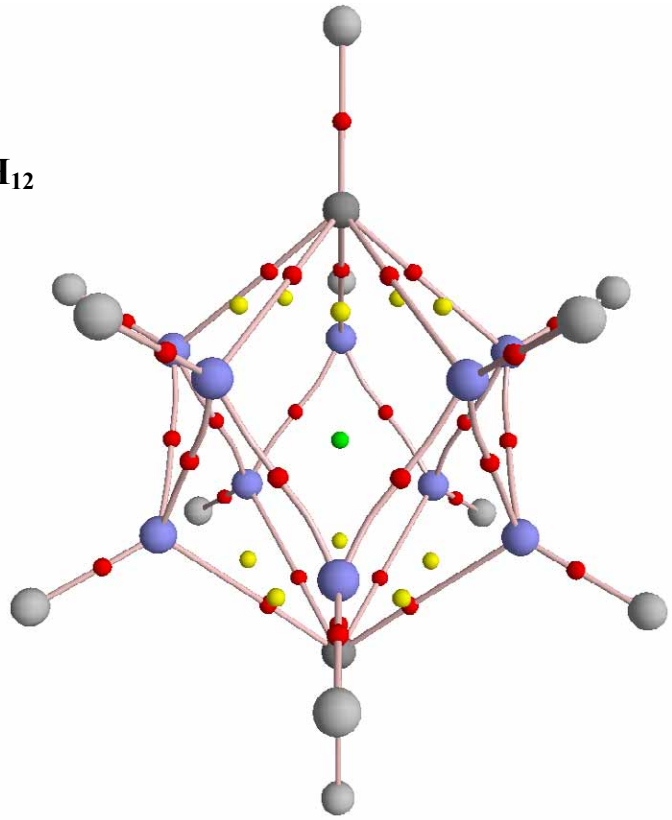


(f)



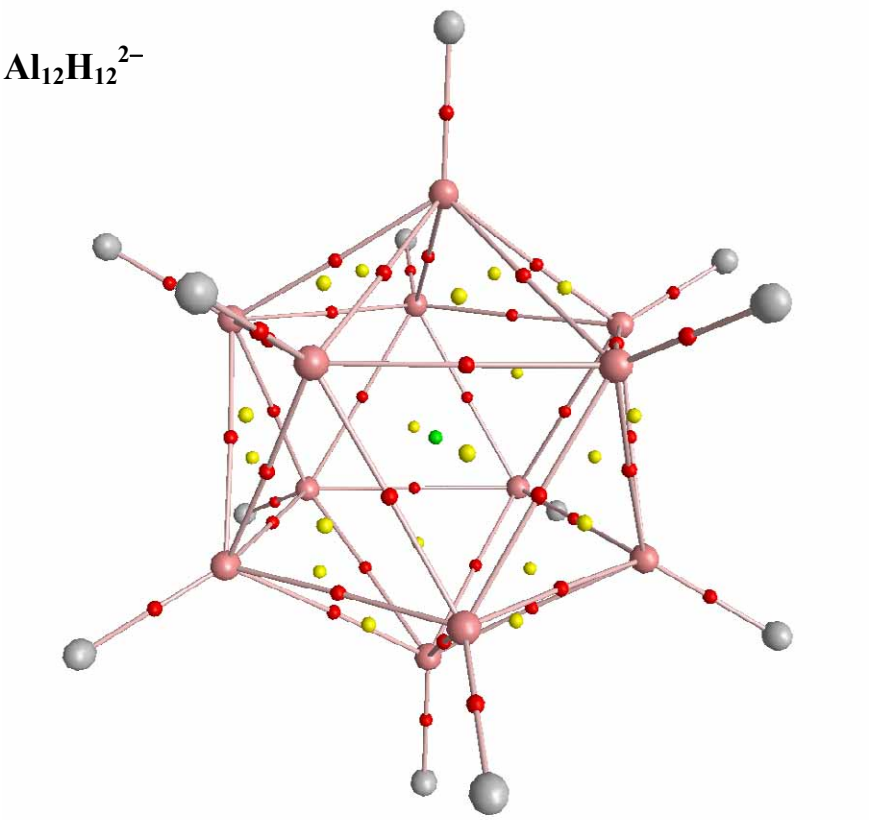
***m*-$Si_2B_{10}H_{12}$**

(g)

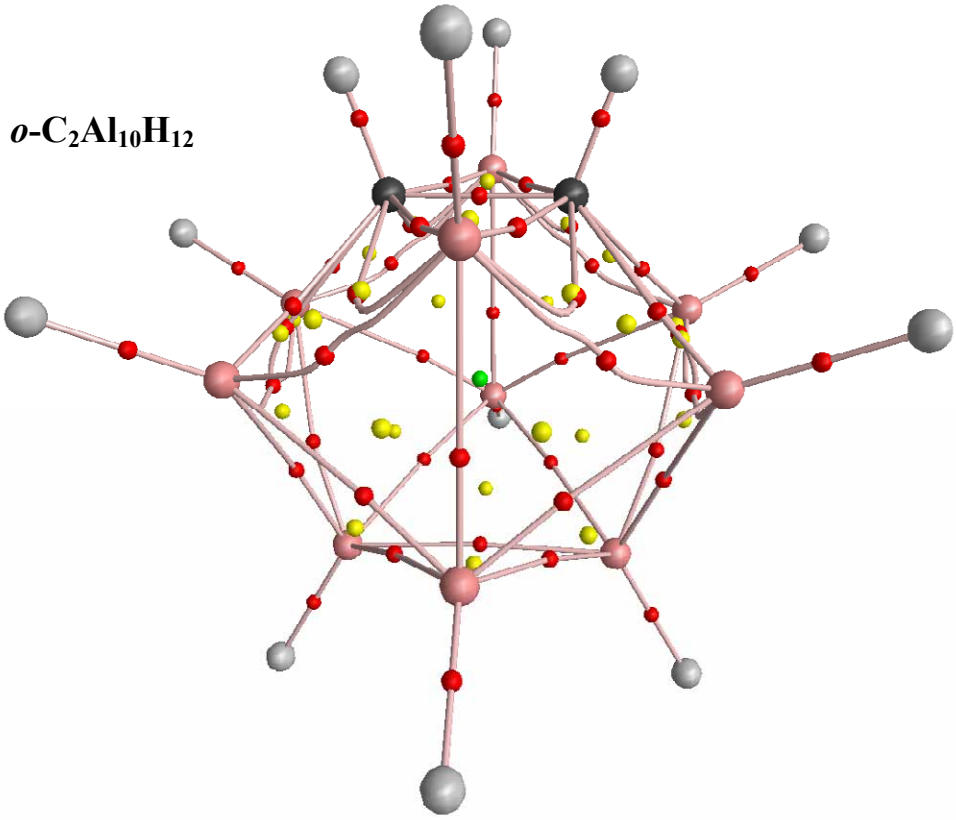


***p*-$Si_2B_{10}H_{12}$**

(h)

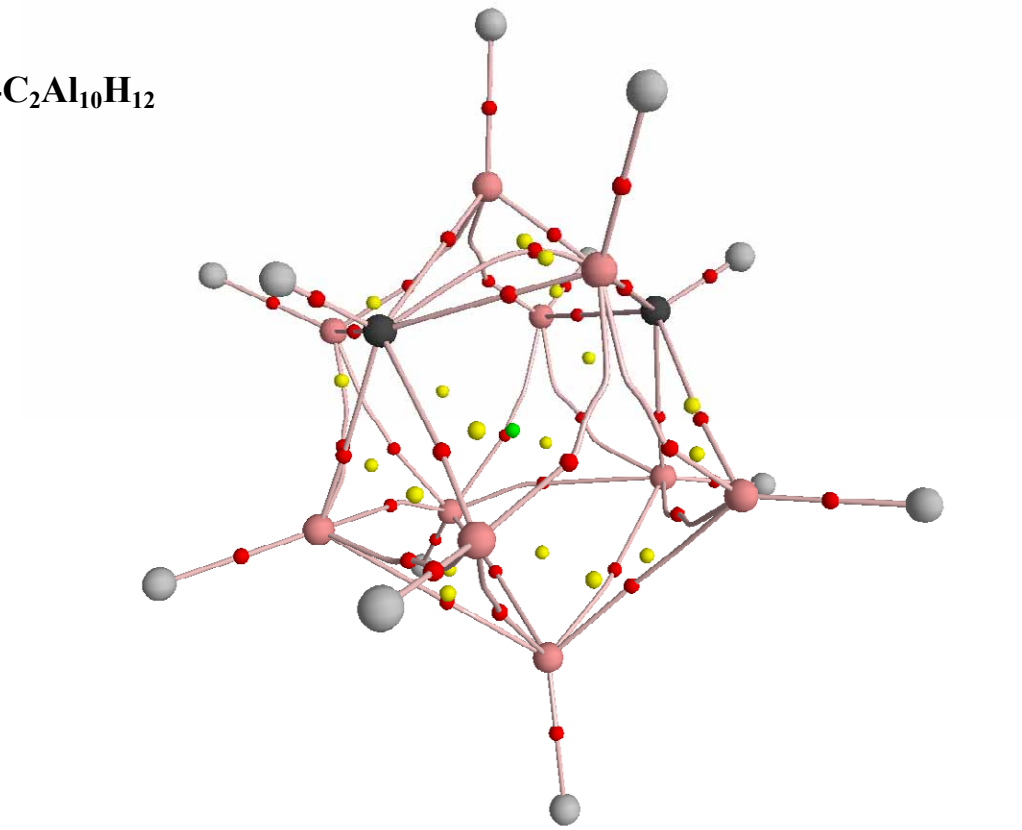


(i)



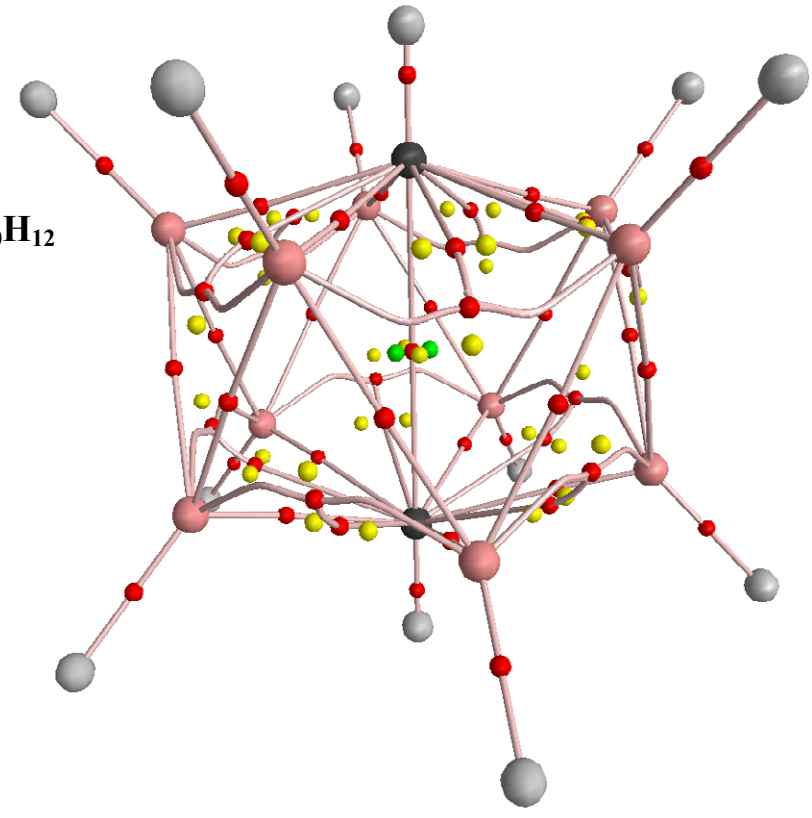
(j)

***m*-$C_2Al_{10}H_{12}$**



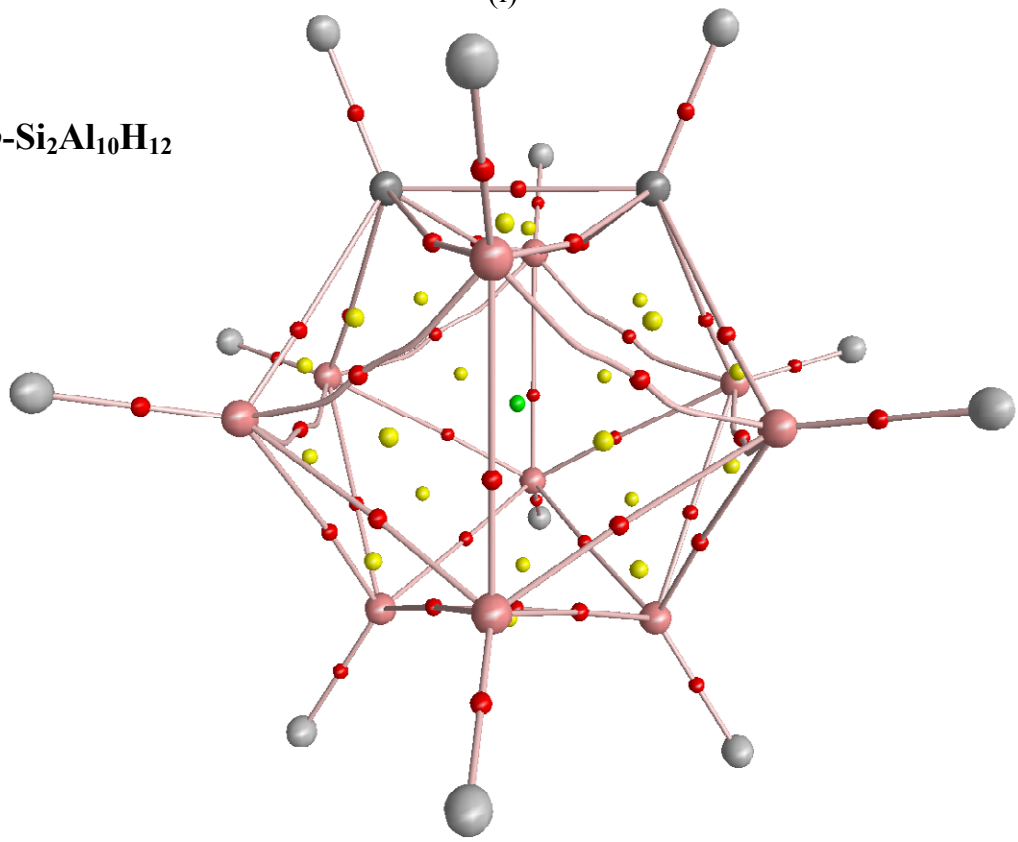
(k)

***p*-$C_2Al_{10}H_{12}$**



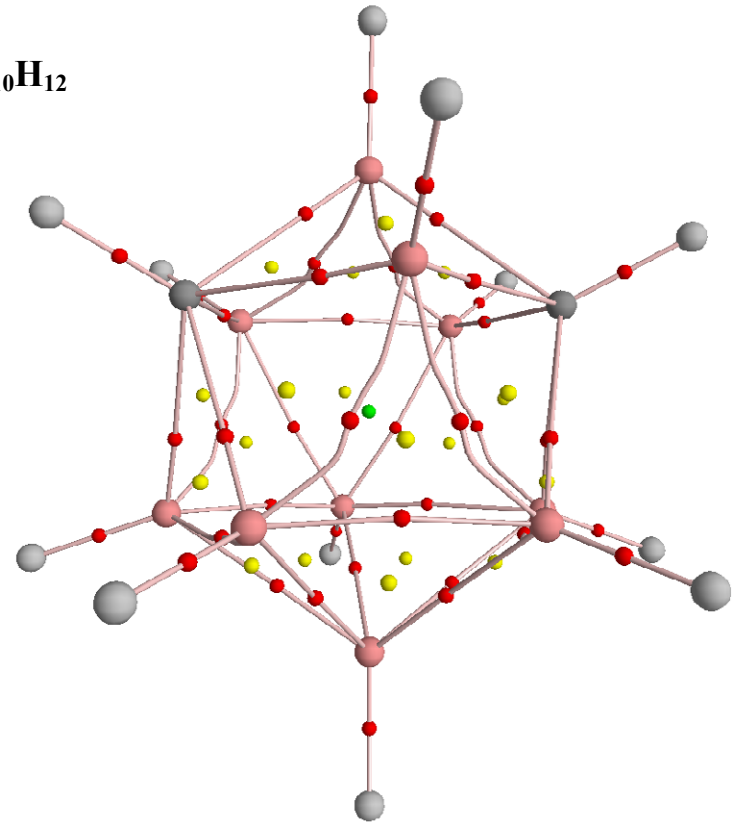
(l)
(l)

***o*-$Si_2Al_{10}H_{12}$**



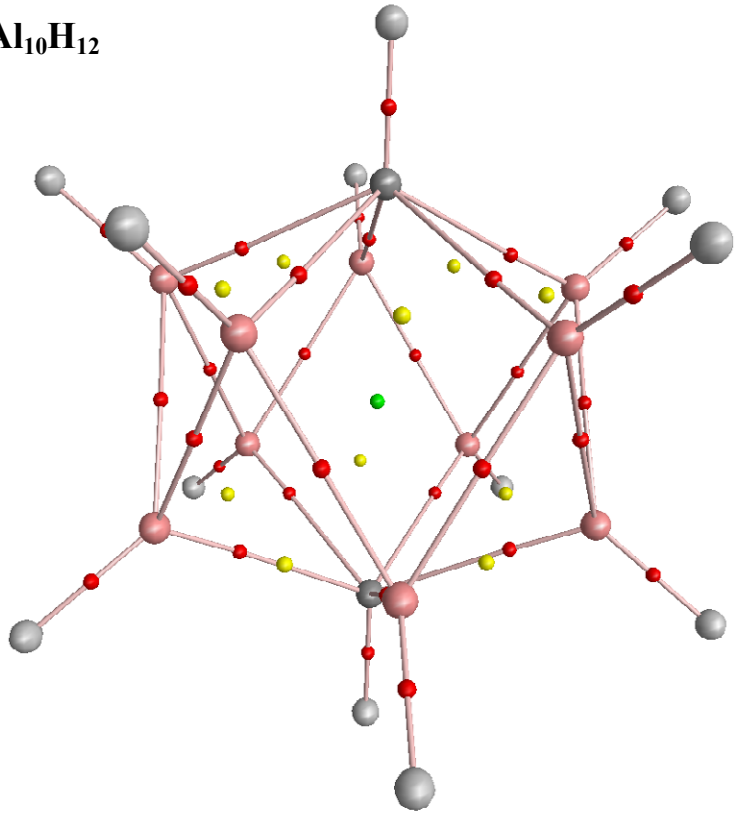
(m)

***m*-$Si_2Al_{10}H_{12}$**



(n)

***p*-$Si_2Al_{10}H_{12}$**



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