Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

$CB_6Al^{0/+}$: Planar Hexacoordinate Boron (phB) in The Global Minimum Structure

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Supporting Information

1. The theoretical background of the methods used

1.1. Gauge-including magnetically induced currents (GIMIC)

For a nucleus K, the nuclear magnetic shielding tensor (σ^K) is proportional to externally applied magnetic field $\boldsymbol{B}$ and nuclear magnetic moment (m^K).[1] Since the surrounding electrons shield the nucleus, each nucleus is coupled differently with the external magnetic field. The expression of Cartesian tensor component ($\sigma^K_{v\tau}$) of σ^K is obtained by Analytical gradient theory,[2] according to which $\sigma^K_{v\tau}$ is the second order derivative of electronic energy with respect to the nuclear magnetic moment (m^K_v) and the Cartesian components of the magnetic field (B_τ) (Equation 1). For the closed-shell system the $\sigma^K_{v\tau}$ is equal to the orbital

$$\sigma^K_{v\tau} = \left[\frac{d^2E}{dm^K_v dB_\tau}\right]_{m^K_v, B_\tau = 0} \qquad (1)$$

contribution ($\sigma^{orbital,K}_{v\tau}$) of the Cartesian shielding tensor as the contact ($\sigma^{contact,K}_{v\tau}$) and dipolar ($\sigma^{dipolar,K}_{v\tau}$) contributions vanish in the case of a closed-shell system.[2] The analytical gradient expression for the orbital contribution of $\sigma^K_{v\tau}$ is given by Equations 2 where $D^{\hbar}_{\mu v}$ and $\frac{\partial D^K_{\mu v}}{\partial B_\tau}$ are the density matrix and magnetically perturbed density

$$\sigma^{orbital,K}_{v\tau} = \sum_{\hbar=\alpha,\beta}\left(\sum_{\mu v} D^{\hbar}_{\mu v}\frac{\partial^2 \hbar_{\mu v}}{\partial m^K_v \partial B_\tau} + \frac{\partial D^K_{\mu v}}{\partial B_\tau}\frac{\partial \hbar_{\mu v}}{\partial m^K_v}\right) \qquad (2)$$

matrices of α and β, electrons, respectively[8]. The derivative terms $\frac{\partial \hbar_{\mu v}}{\partial m^K_v}$ and $\frac{\partial^2 \hbar_{\mu v}}{\partial m^K_v \partial B_\tau}$ represents the external magnetic field and nuclear magnetic moment. The orbital contribution of the αβ electrons to the magnetic shielding tensor can also be expressed in terms of the Biot-Savart law (Equation 3)[3] where $\epsilon_{v\delta\gamma}$ is the Levi-Civita permutation

$$\sigma^{orbital,K}_{v\tau} = \epsilon_{v\delta\gamma}\sum_{\hbar=\alpha,\beta}\int \frac{(r_\delta - R_{K\delta})}{|\boldsymbol{r}-\boldsymbol{R}_K|^3}\frac{\partial \boldsymbol{J}^{\hbar}_{\gamma}(\boldsymbol{r})}{\partial B_\tau} d\boldsymbol{r} \qquad (3)$$

tensor for the Cartesian directions and $\boldsymbol{R}_K$ is the position of nucleus K. It has been assumed that all points in the $\boldsymbol{r}$ space contribute equally to the magnetic interactions. Thus, the expression of the two integrands in Equations 2, and 3 are essentially equal, which gives the value of magnetically induced current densities. When perturbation-dependant GIAOs are used the gauge-origin dependence vanishes (Equation 4) where $\chi_\mu^{(0)}(\boldsymbol{r})$ denotes a standard Gaussian-type function with $\boldsymbol{R}_\mu$ as center and $\boldsymbol{R}_O$ as

$$\chi_\mu(\boldsymbol{r}) = \; e^{-\frac{1}{2}(\boldsymbol{B}\times[\boldsymbol{R}_\mu - \boldsymbol{R}_o]\cdot\boldsymbol{r})}\chi_\mu^{(0)}(\boldsymbol{r}) \qquad (4)$$

the chosen gauge origin. The GIMIC equation (Equation 5) for the calculation of the various magnetically induced current density tensor is obtained by combining

$$J_\nu^{B_\tau,\hbar}(r) = \sum_{\mu\nu} D_{\mu\nu}^{\hbar} \frac{\partial\chi_\mu^*(\boldsymbol{r})}{\partial B_\tau}\frac{\partial\hbar(\boldsymbol{r})}{\partial m_\nu^K}\chi_\nu(\boldsymbol{r}) + \sum_{\mu\nu} D_{\mu\nu}^{\hbar}\,\chi_\mu^*(\boldsymbol{r})\frac{\partial\hbar(\boldsymbol{r})}{\partial m_\nu^K}\frac{\partial\chi_\nu(\boldsymbol{r})}{\partial B_\tau} +$$
$$\sum_{\mu\nu}\frac{\partial D_{\mu\nu}^{\hbar}}{\partial B_\tau}\chi_\mu^*(\boldsymbol{r})\frac{\partial\hbar(\boldsymbol{r})}{\partial m_\nu^K}\chi_\nu(\boldsymbol{r}) - \epsilon_{\nu\delta\gamma}\left[\sum_{\mu\nu} D_{\mu\nu}^{\hbar}\,\chi_\mu^*(\boldsymbol{r})\frac{\partial^2\hbar(\boldsymbol{r})}{\partial m_\nu^K\partial B_\tau}\chi_\nu(\boldsymbol{r})\right] \qquad (5)$$

Equations 2 and 3. Where $J_\nu^{B_\tau,\hbar}(r) = \frac{\partial J_\nu^k(r)}{\partial B_\tau}$ and $\frac{\partial\hbar(\boldsymbol{r})}{\partial m_\nu^K}$, $\frac{\partial^2\hbar(\boldsymbol{r})}{\partial m_\nu^K\partial B_\tau}$ are the nonsingular magnetic interaction operators. For more details, one can read the recent article by Sundholm et al.[1]

1.2. Anisotropy of the magnetically induced current density (ACID)

ACID is a scalar function developed by Herges *et al.*,[4,5] which is used to visualize the electron delocalization in a molecule. The expression of ACID function as given by Herges and Geuenich[5] is as follows:

$$\Delta\mathcal{J}^2(\mathbf{r}) = \frac{1}{3}\left[\left(\mathcal{J}_x^x(\mathbf{r}) - \mathcal{J}_y^y(\mathbf{r})\right)^2 + \left(\mathcal{J}_y^y(\mathbf{r}) - \mathcal{J}_z^z(\mathbf{r})\right)^2 + \left(\mathcal{J}_z^z(\mathbf{r}) - \mathcal{J}_x^x(\mathbf{r})\right)^2\right] + \frac{1}{2}\left[\left(\mathcal{J}_y^x(\mathbf{r}) + \right.\right.$$
$$\left.\left.\mathcal{J}_x^y(\mathbf{r})\right)^2 + \left(\mathcal{J}_z^y(\mathbf{r}) + \mathcal{J}_y^z(\mathbf{r})\right)^2 + \left(\mathcal{J}_x^z(\mathbf{r}) + \mathcal{J}_z^x(\mathbf{r})\right)^2\right] \qquad (6)$$

The ACID function, $\Delta\mathcal{J}^2(\mathbf{r})$ is a scalar function and does not depend on the magnitude and direction of the magnetic field. Thus, it can be used to visualize electron delocalization. However, due to the use of an ordinary basis set, this method suffers from a slow convergence limitation. In the GIMIC code, London atomic orbitals (GIAO) have been used, which makes the convergence of the density matrix, and thereby the ACID function fast.[1] Thus, in this work, the upgraded GIAO-ACID method has been used using the GIMIC method.

The anisotropic component of the current susceptibility is a scalar quantity, like electron density. The scalar component is used to describe the degree of delocalization in a molecule. Since the anisotropic component is used, it is called anisotropy of the magnetically induced current density. Herges and co-workers introduced the original method of ACID analysis.[4] Later it was modified by Sundholm and co-workers by rectifying the slow basis set convergence and positional dependence of the functions. Further the values of the ACID function, $|\Delta\mathcal{J}^2|^{1/2}$ can be grossly used to define the degree of delocalization and hence aromaticity.

Table S1. The values of diatropic (J_{dia}), paratropic (J_{para}), and total current (J_{total}) strengths (nA/T) across various bonds of the local minima within 10 kcal/mol energy of CB_6Al and CB_6Al^+ systems. For atom labeling please see Figure S3.

	Bonds	J_{dia}	J_{para}	J_{total}
CB_6Al (**2a**)	B4−B2	15.73	−0.02	15.71
	B2−B7	16.35	−0.01	16.34
	B7−B3	16.35	−0.01	16.34
	B3−B6	16.84	−0.02	16.82
	B6−C8	17.98	−0.01	17.97
	C8−B4	18.00	−0.02	17.98
CB_6Al (**4a**)	B5−B4	6.62	−0.57	6.05
	B4−B6	5.89	−0.01	5.88
	B6−B7	6.23	−0.81	5.42
	B7−B3	5.84	−0.02	5.82
	B3−B2	5.65	−1.33	4.32
	B2−C8	6.31	−0.92	5.38

	C8−B5	5.94	−0.55	5.39
CB_6Al (**5a**)	B2−B3	6.64	−1.36	5.28
	B3−C8	8.46	−2.55	5.91
	C8−B4	8.29	−3.25	5.04
	B4−B6	7.35	−2.04	5.31
	B6−B5	7.96	−0.78	7.18
	B5−Al1	6.30	−0.60	5.70
	Al1−B2	6.27	−0.67	5.59
CB_6Al^+ (**2b**)	B2−B4	10.32	−0.15	10.16
	B4−B3	10.10	−0.21	9.89
	B3−B6	10.11	−0.21	9.89
	B6−B5	10.32	−0.15	10.16
	B5−C8	10.89	−0.82	10.07
	C8−B2	9.60	−0.95	8.64
CB_6Al^+ (**3b**)	B6−B5	5.23	−4.83	0.39
	B5−B2	5.99	−4.66	1.32
	B2−B4	6.14	−6.54	−0.39
	B4−B7	5.29	−4.72	0.56
	B7−C8	6.04	−8.73	−2.68
	C8−Al1	4.85	−6.15	−1.29
	Al1−B6	4.79	−5.90	−1.10
CB_6Al^+ (**4b**)	B5−B3	3.67	−1.60	2.07
	B3−B6	5.82	−1.39	4.42
	B6−B2	6.06	−1.56	4.49
	B2−B7	5.89	−0.05	5.83
	B7−B4	3.75	−2.42	1.33
	B4−C8	4.89	−1.87	3.01
	C8−B5	3.73	−0.65	3.08

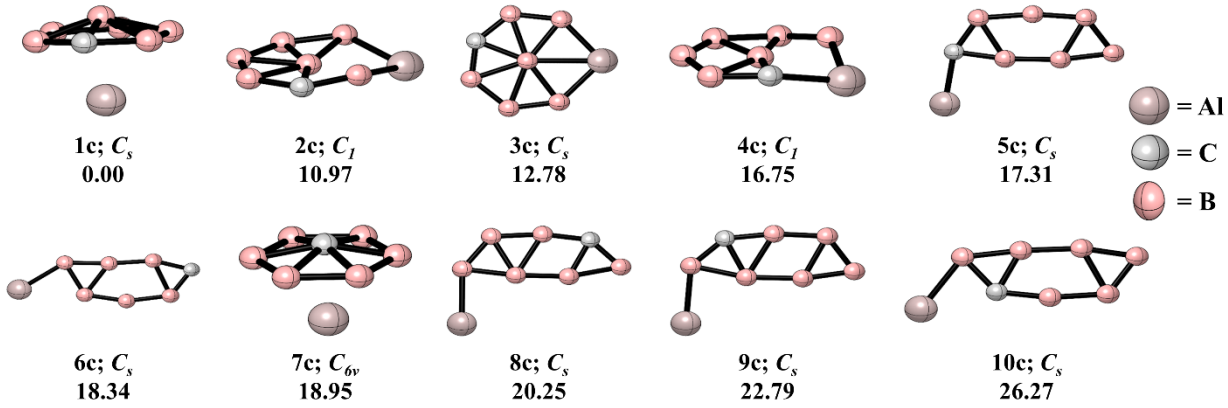

Figure S1. Low-lying isomers of the CB_6Al^- system on the PES. The relative energies are in kcal/mol at PBE0-D3/def2-TZVPP method.

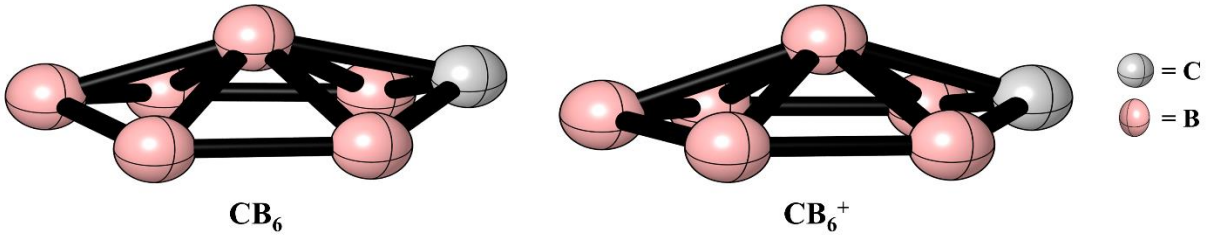

Figure S2. The global minimum structure of CB_6 and CB_6^+ systems at the PBE0-D3/def2-TZVPP method.

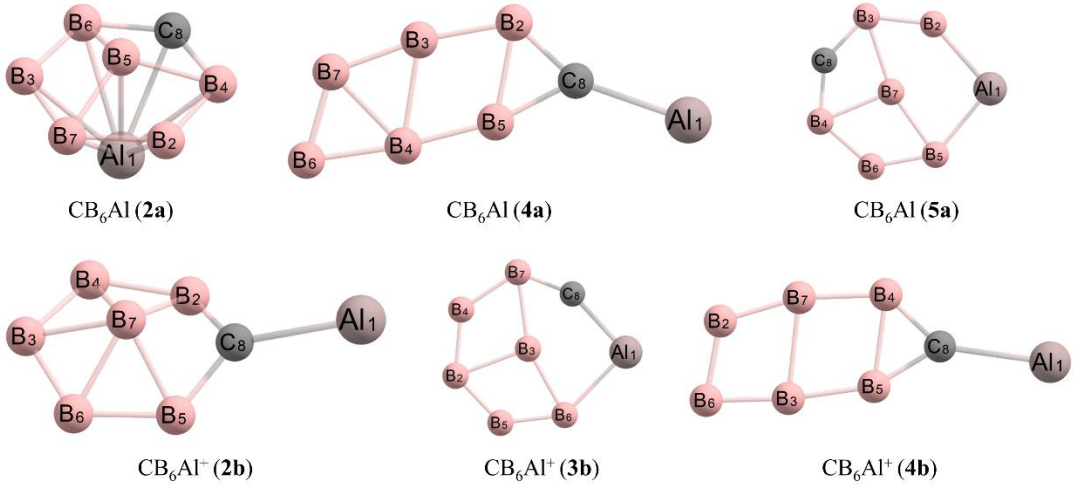

Figure S3. The labeling of the atoms in the considered local minimum structures of CB_6Al and CB_6Al^+ systems.

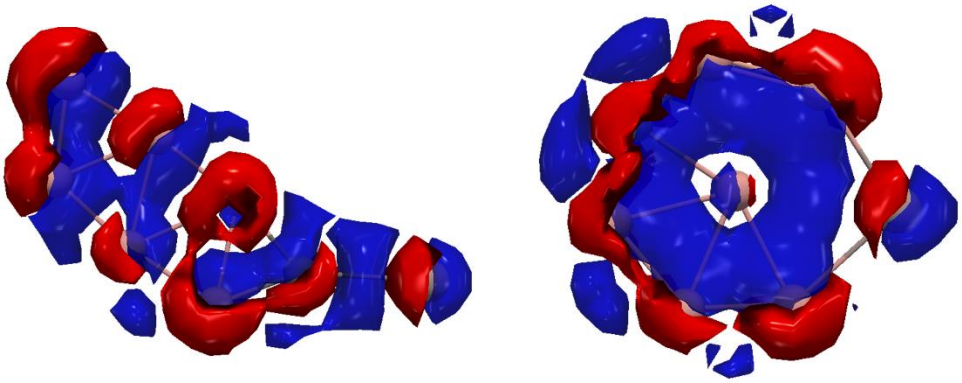

Figure S4. Signed modulus plot of the current density at an isosurface value of 0.03 a.u. for the CB_6Al (**4a**) and CB_6Al (**5a**) which are obtained at the B3LYP/def2-TZVP level. Blue and red components represent the diatropic and paratropic ring current, respectively.

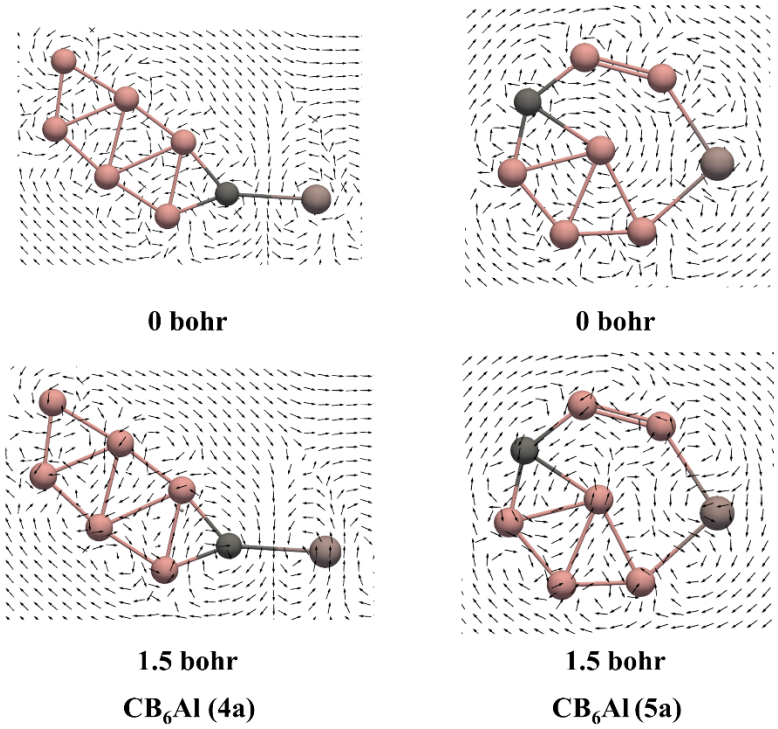

Figure S5. Representation of 2D vector plot of the ring current flow in CB_6Al (**4a**) and CB_6Al (**5a**) on the plane and 1.5 bohr above the molecular plane obtained at the B3LYP/def2-TZVP level of theory. A clockwise vector represents the diatropic ring currents.

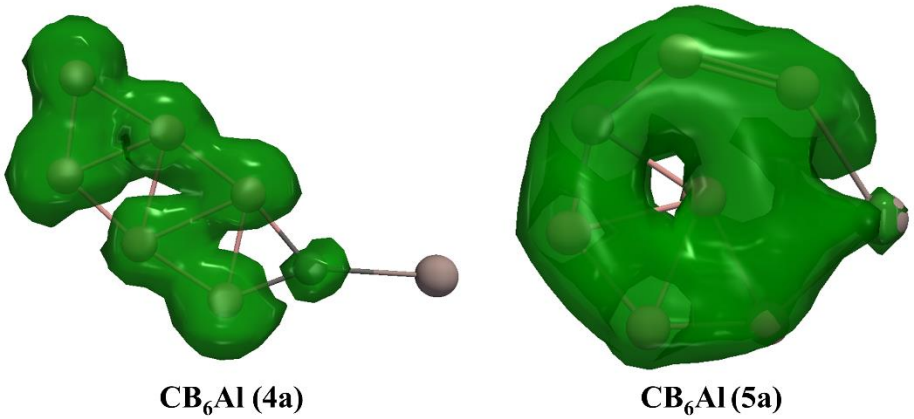

Figure S6. ACID plot at an isosurface value of 0.002 a.u. for CB_6Al (**4a**) and CB_6Al (**5a**) obtained at the B3LYP/def2-TZVP level of theory.

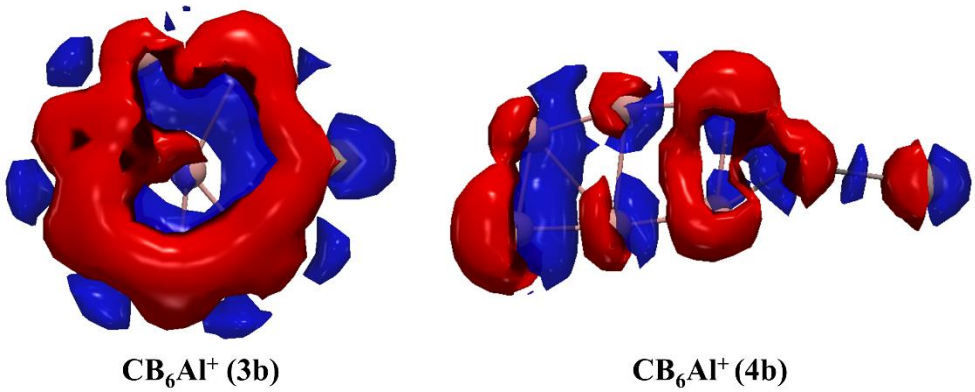

Figure S7. Signed modulus plot of the current density at an isosurface value of 0.03 a.u. for the CB_6Al^+ (**3b**) and CB_6Al^+ (**4b**) which are obtained at the B3LYP/def2-TZVP level. Blue and red components represent the diatropic and paratropic ring current, respectively.

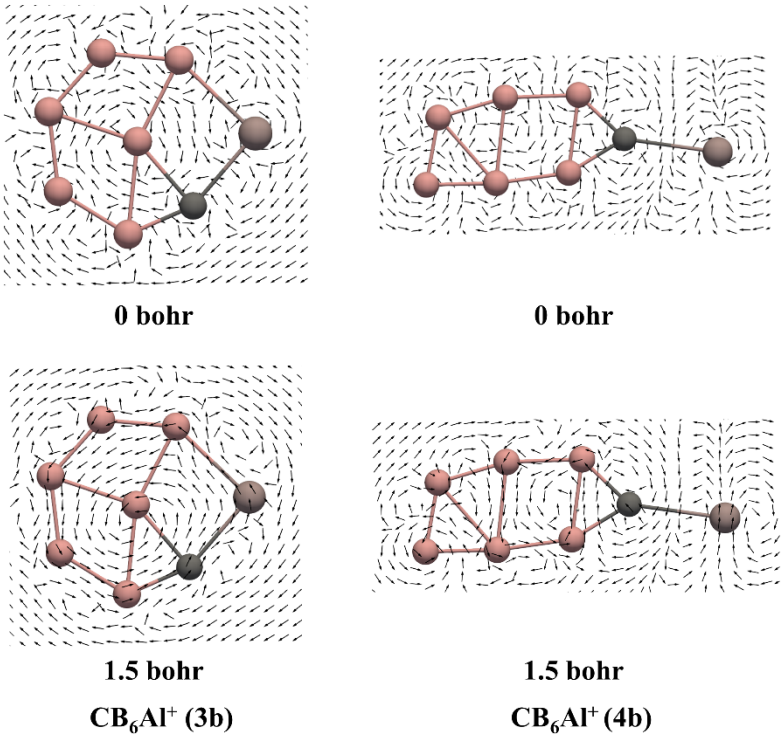

Figure S8. Representation of 2D vector plot of the ring current flow in CB_6Al^+ (**3b**) and CB_6Al^+ (**4b**) on the plane and 1.5 bohr above the molecular plane obtained at the B3LYP/def2-TZVP level of theory. A clockwise vector represents the diatropic ring currents.

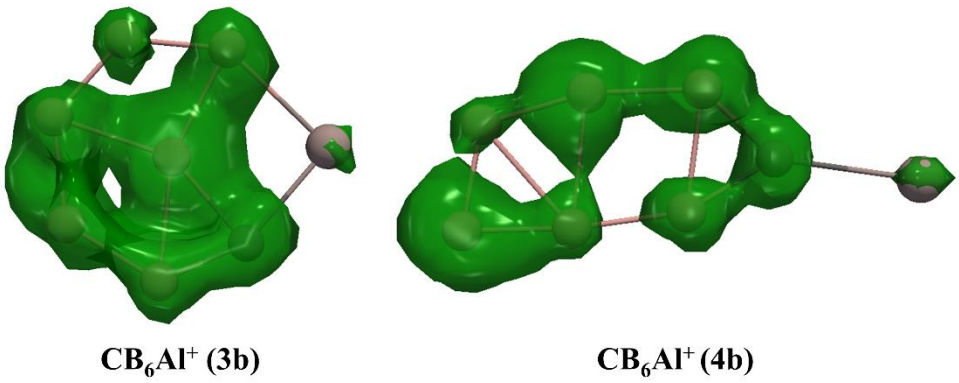

Figure S9. ACID plot at an isosurface value of 0.002 a.u. for CB_6Al^+ (**3b**) and CB_6Al^+ (**4b**) obtained at the B3LYP/def2-TZVP level of theory.

Coordinates of the optimized geometries

	1a		
Al	-0.31456200	-1.90130400	0.00000000
B	-1.61652400	1.14593700	0.00000000
B	0.00000000	0.40321700	0.00000000
B	-0.44605600	2.13977000	0.00000000
B	-1.57144100	-0.37646100	0.00000000
B	1.36644100	-0.82689400	0.00000000
B	1.07300500	1.81827000	0.00000000
C	1.67702900	0.53296000	0.00000000
	2a		
Al	-1.24030700	0.04812600	0.00000000
B	0.36759000	0.79084200	1.38539200
B	0.36759000	0.79084200	-1.38539200
B	0.36759000	-0.80379900	1.33038900
B	0.92624800	0.03887100	0.00000000
B	0.36759000	-0.80379900	-1.33038900
B	0.37233100	1.60466000	0.00000000
C	0.37988300	-1.45228800	0.00000000
	3a		
Al	-1.35950900	0.61035100	0.00000700
B	0.96560400	-0.52500400	0.00015800
B	0.03414500	-0.91271500	1.35292600
B	0.71252100	0.54418000	1.28137500
B	0.03613800	-0.90736400	-1.35613300
B	0.71566700	0.54889700	-1.27843900
B	-0.28459400	-1.64501700	-0.00319000
C	1.12936700	1.09175900	0.00273700
	4a		
Al	2.94750700	-0.85811000	0.00000000
B	-0.35528200	-1.23407100	0.00000000
B	-1.69885700	-0.35821400	0.00000000
B	-1.26553100	1.37490600	0.00000000
B	0.00000000	0.41300800	0.00000000
B	-2.65580500	2.21638100	0.00000000
B	-2.84692700	0.70259500	0.00000000
C	0.96573600	-0.73626500	0.00000000

5a			
Al	-0.26204100	-1.91088700	0.00000000
B	1.40519800	-0.83897900	0.00000000
B	1.80637500	0.66063000	0.00000000
B	-0.43912400	2.06576700	0.00000000
B	-1.58144400	-0.44767300	0.00000000
B	-1.63743400	1.05616500	0.00000000
B	0.00000000	0.35339700	0.00000000
C	0.93977900	1.76583300	0.00000000
6a			
Al	-0.19533300	-1.85420100	0.00000000
B	1.00083500	1.92764500	0.00000000
B	-1.67300100	1.09230000	0.00000000
B	-0.52143500	2.11420300	0.00000000
B	-1.58534600	-0.42014500	0.00000000
B	1.79136000	0.57298800	0.00000000
B	0.00000000	0.38198800	0.00000000
C	1.24621000	-0.70671400	0.00000000
7a			
Al	0.00000000	0.00000000	1.77737300
B	0.00000000	1.32267500	-1.21596900
B	0.86772500	0.00000000	-0.33822700
B	0.00000000	-1.32267500	-1.21596900
B	0.00000000	-1.40177500	0.33191500
B	-0.86772500	0.00000000	-0.33822700
B	0.00000000	1.40177500	0.33191500
C	0.00000000	0.00000000	-1.81384000
8a			
Al	0.04745000	1.78612900	0.00000000
B	-1.40235000	-1.19660300	0.00000000
B	-0.03842700	-1.94405000	0.00000000
B	1.36115100	0.27135800	0.00000000
B	-0.03842700	-0.36486200	0.87536200
B	-1.38991400	0.35418400	0.00000000
B	-0.03842700	-0.36486200	-0.87536200
C	1.18585300	-1.16591800	0.00000000
9a			
Al	0.02416300	1.75297500	0.00000000
B	-0.04874300	-1.98263900	0.00000000

B	1.35072800	-1.29598600	0.00000000
B	0.02416300	-0.37541600	0.87059300
B	1.40516700	0.25213900	0.00000000
B	0.02416300	-0.37541600	-0.87059300
B	-1.35609300	-1.13950000	0.00000000
C	-1.21850800	0.29923500	0.00000000
10a			
Al	3.19275900	-0.82788500	0.00000000
B	-2.71591600	2.10168700	0.00000000
B	1.04116500	-0.85856500	0.00000000
B	-0.41408500	-1.28331600	0.00000000
B	0.00000000	0.35077400	0.00000000
B	-1.26091100	1.36800200	0.00000000
B	-1.71363700	-0.36666300	0.00000000
C	-2.69815800	0.70048500	0.00000000
11a			
Al	-2.59863900	-1.20486800	0.00000000
B	1.51577200	1.44564300	0.00000000
B	-1.52479800	0.44644800	0.00000000
B	2.56505800	0.09280400	0.00000000
B	-0.43237500	-0.78992200	0.00000000
B	1.11118100	-0.61634200	0.00000000
B	0.00000000	0.83968400	0.00000000
C	2.93468700	1.42861900	0.00000000
12a			
Al	1.62515100	1.79535100	0.00000000
B	-1.56558200	-0.66928500	0.00000000
B	-1.55078800	0.89795100	0.00000000
B	0.29317100	-1.38222600	0.00000000
B	0.00000000	0.22075800	0.00000000
B	-1.16431300	-2.23201700	0.00000000
B	-0.36289900	1.85915200	0.00000000
C	0.10418100	-2.80187200	0.00000000
13a			
Al	1.65907900	-0.88965800	-0.12311600
B	-0.49477900	-1.22202500	0.08367100
B	-1.79567700	0.01596200	-0.11483600
B	0.18755200	2.06715200	-0.02520200
B	1.41238100	1.15773300	0.20088900

B	-1.26620300	1.53925500	-0.23432800
B	-0.06955400	0.44364900	0.31138700
C	-1.90610400	-1.40717900	0.08210000
	14a		
Al	-2.26632500	0.04275300	-0.21679700
B	1.04330500	1.50707600	0.26794100
B	-0.43838100	0.87033700	0.47604400
B	0.76411700	-1.47006800	0.31505800
B	2.13973100	-0.85280800	-0.20209400
B	0.72066700	0.01803100	-0.43704900
B	2.26914900	0.68609300	-0.27720600
C	-0.50512000	-0.72485000	0.35081800
	15a		
Al	1.74923700	-0.88729500	-0.13162000
B	0.24497800	1.91725500	-0.04804600
B	-1.87640400	0.06637300	-0.10170400
B	-0.15414100	0.31245300	0.24723800
B	-1.30113300	1.53747900	-0.22541400
B	-0.72916400	-1.20921500	0.12340000
B	-2.23878300	-1.50406700	0.05179900
C	1.25552500	0.98890800	0.24578300
	16a		
Al	1.71713600	-0.89051200	-0.12924900
B	-0.16922000	0.33500400	0.29947200
B	-0.55490800	-1.24383200	0.11706100
B	-1.29070100	1.47112600	-0.27147300
B	-1.79684900	-0.06558200	-0.12407900
B	-2.05623600	-1.63359200	0.08644400
B	1.30882500	1.21308300	0.22687800
C	0.07877800	1.86593800	0.00145300
	17a		
Al	-0.80805100	2.33427000	0.00000000
B	1.02237600	1.57366800	0.00000000
B	0.00000000	0.24576400	0.00000000
B	-1.14652300	-2.74877600	0.00000000
B	1.70390400	0.20673200	0.00000000
B	-0.77759800	-1.20091500	0.00000000
B	1.05153700	-1.22942600	0.00000000
C	0.20603000	-2.43012400	0.00000000

18a			
Al	-2.25128900	-0.04318300	0.24903000
B	0.94274500	-1.46936200	-0.32104300
B	0.59567500	0.04050900	0.33861200
B	-0.55722900	-0.84420900	-0.51704700
B	2.11935200	0.70683900	0.19970500
B	0.84961100	1.61277700	-0.17231900
B	-0.51339600	0.93490200	-0.53293900
C	2.01382800	-0.72431700	0.29796200
19a			
Al	0.08051000	0.00021800	0.85620700
B	1.64312200	0.78852400	-0.32957600
B	1.64087400	-0.79150500	-0.32984000
B	-1.10692100	1.25590700	-0.37091800
B	0.41324200	1.75677700	-0.31532700
B	0.40978800	-1.75815600	-0.31490500
B	-1.10929500	-1.25399200	-0.37063500
C	-1.75011300	0.00156500	-0.16244800
20a			
Al	-1.12667600	0.29430900	0.00000000
B	0.57951000	0.33237200	1.48138400
B	0.57951000	1.68740700	0.76956200
B	0.57951000	1.68740700	-0.76956200
B	0.35007600	-1.17612700	1.02082100
B	0.35007600	-1.17612700	-1.02082100
B	0.57951000	0.33237200	-1.48138400
C	-0.07402800	-2.04375600	0.00000000
21a			
Al	1.70909300	-1.05090000	0.00000000
B	-0.88424500	1.17617800	1.17500400
B	-0.88424500	-0.37941300	1.01608000
B	-0.88424500	1.17617800	-1.17500400
B	0.28840100	0.54341800	0.00000000
B	-0.88424500	-0.37941300	-1.01608000
B	-0.73780500	2.15899900	0.00000000
C	-0.38104900	-1.30300700	0.00000000
22a			
Al	1.57314000	-0.87815600	-0.16642000
B	1.35296500	1.17896700	0.29870300

B	-0.12280300	0.43283600	0.33797000
B	-1.74376300	-0.03655700	-0.16656000
B	-1.83802200	-1.60799100	0.16178600
B	-1.27414000	1.51719100	-0.30544100
B	0.14849900	2.08064800	-0.01507200
C	-0.51075100	-1.06824100	0.10108800
23a			
Al	-1.56771700	-1.14748300	0.00000000
B	0.83389200	1.17365200	1.07711600
B	0.83389200	1.17365200	-1.07711600
B	0.83389200	-0.40335500	1.01138300
B	0.54057200	-1.56044800	0.00000000
B	-0.36680400	0.52547500	0.00000000
B	0.83389200	-0.40335500	-1.01138300
C	0.47227400	2.06486200	0.00000000
24a			
Al	-1.86221000	-0.59848300	-0.10796400
B	0.19217600	0.64107700	1.08074500
B	2.17146000	-0.85035400	-0.10893600
B	-0.99018000	1.26982400	0.25021800
B	0.18586700	1.13042100	-0.79448300
B	0.20474100	-0.60642700	-0.21372700
B	1.47601700	0.24792200	-1.01891900
C	1.33472000	-0.23033900	0.90484100
25a			
Al	1.81232300	-0.03924200	-0.50374100
B	-0.22742400	1.18748000	0.76837700
B	-0.27603500	0.00342900	-0.65745600
B	-1.32833300	1.38580100	-0.34322900
B	-0.24366300	-1.00415400	0.86721500
B	0.80586500	0.09910300	1.29401800
B	-1.96185300	-0.04879700	-0.43337700
C	-1.23383200	-1.26736000	-0.15485100
26a			
Al	0.08051000	0.00021800	0.85620700
B	1.64312200	0.78852400	-0.32957600
B	1.64087400	-0.79150500	-0.32984000
B	-1.10692100	1.25590700	-0.37091800
B	0.41324200	1.75677700	-0.31532700

B	0.40978800	-1.75815600	-0.31490500
B	-1.10929500	-1.25399200	-0.37063500
C	-1.75011300	0.00156500	-0.16244800
	27a		
Al	2.16625600	-0.00892200	0.01644500
B	-2.31078300	-0.01549800	-0.53002600
B	-0.34532500	-0.01312700	0.93210300
B	0.45344900	1.09243000	-0.12665700
B	-1.08904300	1.02662000	-0.44708100
B	-0.95090300	-0.87700900	-0.58068500
B	-1.92344200	-0.13852400	0.96813400
C	0.44481800	-0.87641100	-0.21545500
	28a		
Al	-0.70893600	1.16931700	-0.33946000
B	-1.70763400	-0.63536300	-0.24913300
B	0.50011900	-0.33055900	0.86641000
B	1.76825000	0.09407500	-0.25777200
B	-1.00360800	-0.79352000	1.10415400
B	1.17181200	1.32338600	0.52791300
B	-0.27401700	-1.28855700	-0.51986300
C	1.15692600	-1.17473800	-0.49092900
	1b		
Al	-0.32783600	-1.94426200	0.00000000
B	0.00000000	0.43206800	0.00000000
B	1.39491900	-0.81623000	0.00000000
B	-1.57158500	-0.34656600	0.00000000
B	-0.46100400	2.14923700	0.00000000
B	-1.64045400	1.17048700	0.00000000
B	1.09762900	1.82214200	0.00000000
C	1.69405800	0.53662000	0.00000000
	2b		
Al	0.89351400	2.61292400	0.00000000
B	-0.54651700	-0.16777700	1.13182900
B	-0.39756500	-2.64118300	0.00000000
B	-0.54651700	-1.75953200	1.27032500
B	-0.54651700	-0.16777700	-1.13182900
B	-0.54651700	-1.75953200	-1.27032500
B	0.32035000	-1.06843000	0.00000000
C	-0.04987700	0.64219200	0.00000000

3b			
Al	0.15523700	-1.89303300	0.00000000
B	0.57936400	2.12325000	0.00000000
B	0.00000000	0.40112000	0.00000000
B	-0.97278700	1.93874300	0.00000000
B	1.71921100	1.10580100	0.00000000
B	1.58357100	-0.41037400	0.00000000
B	-1.80722000	0.58204600	0.00000000
C	-1.25479600	-0.68225000	0.00000000
4b			
Al	-3.15997901	-0.17285083	0.00000000
B	2.99647402	0.58620492	0.00000000
B	1.72615797	-0.85903103	0.00000000
B	-0.09462696	1.08480704	0.00000000
B	0.12670098	-0.63229696	0.00000000
B	3.26076096	-0.89663409	0.00000000
B	1.52468804	1.02720898	0.00000000
C	-1.10350800	0.11596108	0.00000000
5b			
Al	1.71242600	-0.14117000	0.00000000
B	-1.27300900	-0.05784200	0.00000000
B	-0.41014400	0.85188300	1.15724500
B	-0.41014400	-0.77996000	-1.26261900
B	-0.41014400	0.85188300	-1.15724500
B	-0.60580100	-1.65242300	0.00000000
B	-0.41014400	-0.77996000	1.26261900
C	-0.77743400	1.61122000	0.00000000
6b			
Al	-1.71016700	-1.09678700	0.00000000
B	-0.16186800	0.61997900	0.00000000
B	0.85030200	-0.37277800	1.06417100
B	0.85030200	-0.37277800	-1.06417100
B	0.80716200	2.09121600	0.00000000
B	0.85030200	1.19116400	1.26762800
B	0.85030200	1.19116400	-1.26762800
C	0.33327900	-1.24693200	0.00000000
7b			
Al	0.33353100	-1.95611700	0.00000000
B	-1.39047700	-0.83361800	0.00000000

B	0.00000000	0.37083200	0.00000000
B	1.62098800	1.08233400	0.00000000
B	0.39288300	2.08491800	0.00000000
B	-1.86557400	0.68244800	0.00000000
B	1.57868000	-0.41936300	0.00000000
C	-1.00306700	1.76529400	0.00000000
8b			
Al	-2.25312100	-0.08747100	-0.19961400
B	0.74416200	1.47385500	0.30219800
B	2.27175300	-0.70430700	-0.26766900
B	2.12970800	0.84191400	-0.13816000
B	-0.35661100	-0.80141800	0.57247300
B	0.69472300	-0.01319400	-0.51735100
B	1.03726300	-1.50560200	0.24227100
C	-0.55240200	0.78014700	0.27103100
9b			
Al	1.12841300	1.01153000	-0.21703200
B	-0.86638200	1.34016400	0.23648000
B	1.54431700	-0.97336700	-0.25804900
B	0.71662500	-0.98999300	1.04695200
B	0.04712900	-1.36649100	-0.57930200
B	-1.45175700	-0.80182700	-0.67314400
B	-0.66476400	-0.31986700	0.84552600
C	-1.88253700	0.40117000	-0.04515100
10b			
Al	3.26400100	-0.69874200	0.00000000
B	0.00000000	0.52414400	0.00000000
B	1.11366300	-0.54027100	0.00000000
B	-2.92504200	1.76692400	0.00000000
B	-1.42808400	1.34708300	0.00000000
B	-1.69278400	-0.57130200	0.00000000
B	-0.23737000	-1.19558200	0.00000000
C	-2.76398800	0.40477700	0.00000000
11b			
Al	3.05234400	-1.49563500	0.00000000
B	-1.70739000	-0.06772900	0.00000000
B	-1.16692000	1.73631300	0.00000000
B	-2.87634300	0.96622200	0.00000000
B	-2.53403100	2.42494900	0.00000000

B	0.91080100	-0.75529800	0.00000000
B	0.00000000	0.62188100	0.00000000
C	-0.46850900	-0.86473800	0.00000000
	12b		
Al	-0.80630200	1.26343500	-0.13350600
B	-1.75346900	-0.54646100	-0.05353800
B	-0.50106500	-0.80333500	0.93281900
B	-0.76333900	-1.57099300	-0.58096100
B	0.79215500	-1.25678300	-0.33212700
B	0.89477200	-0.07256000	0.94236300
B	1.28476400	1.14662500	-0.14480800
C	1.78547300	-0.15118700	-0.34719300
	13b		
Al	-0.69060000	1.24734800	-0.14866300
B	1.92319000	-0.25475200	-0.45638900
B	-0.82107200	-1.42361300	-0.58748800
B	0.77967100	-1.34505100	-0.30129200
B	-0.45879400	-0.72629700	0.90819100
B	1.36195200	1.11789000	-0.11518000
B	0.98075600	-0.09528900	0.94488000
C	-1.64178800	-0.42999600	-0.00516400
	14b		
Al	-2.17306400	-0.01629400	-0.23560400
B	0.91816700	-1.50879100	0.28563000
B	0.85275600	1.59762500	0.22985000
B	2.11222100	0.73650300	-0.20819300
B	-0.57863300	-0.94724400	0.48826700
B	-0.58241700	0.96610500	0.50655100
B	0.55208100	0.01591300	-0.41536900
C	1.97982600	-0.68145600	-0.22847100
	15b		
Al	1.79519000	-0.52054600	-0.27953600
B	-0.26659400	-0.58612600	-0.37989600
B	-1.42488900	0.53604800	-1.09256300
B	-0.16254800	1.29321400	-0.47643000
B	-2.07023700	-0.62100200	-0.28084000
B	0.96459500	1.15370700	0.61409500
B	-0.17424200	0.28002800	1.25849400
C	-1.27798300	-0.58537400	0.90327700

16b			
Al	1.09105400	1.04647900	-0.25124300
B	-0.87968700	1.36732100	0.27849900
B	-0.04830300	-1.35535500	-0.56901700
B	-2.08179500	0.48315900	-0.04022900
B	-1.54207600	-0.83278000	-0.63336700
B	-0.61081200	-0.25642800	0.79195300
B	1.50958800	-0.98810200	-0.25081500
C	0.68028700	-0.94888300	0.89683800
17b			
Al	-0.92500600	0.21197600	0.00000000
B	0.51837500	0.35355500	1.60185300
B	0.27148600	-1.18820500	-1.15767700
B	0.27148600	-1.18820500	1.15767700
B	0.51837500	1.67408700	0.77753700
B	0.51837500	1.67408700	-0.77753700
B	0.51837500	0.35355500	-1.60185300
C	-0.17621100	-1.85834500	0.00000000
18b			
Al	1.00916200	1.08789500	-0.21493600
B	-2.07506100	0.31296800	-0.10652000
B	1.60328600	-0.86826600	-0.29186900
B	0.09618200	-1.17722700	-0.66045100
B	0.83520800	-1.07293100	1.02795200
B	-0.95407400	1.25868500	0.40201100
B	-0.57185900	-0.36680100	0.88562700
C	-1.29791800	-0.76246200	-0.58159700
19b			
Al	1.51126500	-1.10203400	0.00000000
B	-0.77575700	-0.41549700	1.08234500
B	0.39441900	0.59543000	0.00000000
B	-0.77575700	1.16470100	1.19859700
B	-0.53679200	-1.52466200	0.00000000
B	-0.77575700	-0.41549700	-1.08234500
B	-0.77575700	1.16470100	-1.19859700
C	-0.56990600	1.91342900	0.00000000
20b			
Al	3.19725200	-0.87040800	0.00000000
B	1.05362800	-0.64531700	0.00000000

B	-2.82411600	0.55248800	0.00000000
B	-1.77037200	-0.66055800	0.00000000
B	-1.29862500	1.49718700	0.00000000
B	-0.31535800	-1.25578000	0.00000000
B	0.00000000	0.48240200	0.00000000
C	-2.63167700	1.91053300	0.00000000

1c

Al	1.397189000000	0.001936000000	0.000000000000
B	-0.972082000000	0.062180000000	0.000000000000
B	-0.418596000000	-0.782642000000	1.321465000000
B	-0.414515000000	1.611413000000	0.000000000000
B	-0.418596000000	0.806788000000	-1.383768000000
B	-0.418596000000	0.806788000000	1.383768000000
B	-0.418596000000	-0.782642000000	-1.321465000000
C	-0.476425000000	-1.439100000000	0.000000000000

2c

Al	1.929862000000	0.025697000000	-0.137905000000
B	0.610405000000	-1.446107000000	0.271600000000
B	-2.049998000000	0.761052000000	-0.088570000000
B	-1.959544000000	-0.779496000000	-0.056694000000
B	-0.431096000000	0.059990000000	-0.021318000000
B	0.611445000000	1.466607000000	0.301608000000
B	-0.874904000000	1.749789000000	-0.027489000000
C	-0.769957000000	-1.565539000000	-0.017154000000

3c

Al	-0.124208000000	-1.897867000000	0.000000000000
B	-1.559598000000	-0.534645000000	0.000000000000
B	-1.705826000000	0.970374000000	0.000000000000
B	1.739582000000	0.733543000000	0.000000000000
B	0.000000000000	0.324222000000	0.000000000000
B	-0.579139000000	2.032228000000	0.000000000000
B	1.459487000000	-0.766197000000	0.000000000000
C	0.807028000000	1.812440000000	0.000000000000

4c

Al	1.855579000000	0.013825000000	-0.140127000000
B	0.601649000000	1.526567000000	0.325347000000
B	-2.026859000000	-0.792387000000	-0.043835000000
B	-0.857690000000	1.746584000000	-0.085961000000
B	-0.766501000000	-1.702211000000	-0.009287000000

B	-0.420474000000	0.023707000000	0.011466000000
B	-2.034766000000	0.735288000000	-0.084950000000
C	0.566780000000	-1.311244000000	0.209624000000
		5c	
Al	-0.090243000000	2.538215000000	0.000000000000
B	-0.572674000000	-1.612042000000	0.000000000000
B	0.626481000000	-2.628312000000	0.000000000000
B	2.114479000000	-2.283918000000	0.000000000000
B	-1.613611000000	-0.376622000000	0.000000000000
B	0.000000000000	0.117553000000	0.000000000000
B	1.176491000000	-1.020393000000	0.000000000000
C	-1.247112000000	1.003645000000	0.000000000000
		6c	
Al	1.915005000000	-2.339689000000	0.000000000000
B	0.322571000000	0.785952000000	0.000000000000
B	-2.296822000000	1.278277000000	0.000000000000
B	1.524887000000	-0.303753000000	0.000000000000
B	0.000000000000	-0.849093000000	0.000000000000
B	-0.767069000000	1.990966000000	0.000000000000
B	-1.300331000000	-0.001262000000	0.000000000000
C	-2.051874000000	2.651754000000	0.000000000000
		7c	
Al	0.000000000000	0.000000000000	1.404196000000
B	0.000000000000	1.578512000000	-0.445501000000
B	-1.367031000000	-0.789256000000	-0.445501000000
B	-1.367031000000	0.789256000000	-0.445501000000
B	1.367031000000	-0.789256000000	-0.445501000000
B	0.000000000000	-1.578512000000	-0.445501000000
B	1.367031000000	0.789256000000	-0.445501000000
C	0.000000000000	0.000000000000	-0.814920000000
		8c	
Al	1.478063000000	2.194411000000	0.000000000000
B	-1.373631000000	-0.963587000000	0.000000000000
B	-0.570829000000	1.733044000000	0.000000000000
B	0.360942000000	-3.040419000000	0.000000000000
B	-1.616620000000	0.598609000000	0.000000000000
B	0.000000000000	0.181470000000	0.000000000000
B	0.385192000000	-1.398755000000	0.000000000000
C	-0.856681000000	-2.346524000000	0.000000000000

	9c		
Al	-0.084893000000	2.605137000000	0.000000000000
B	0.644047000000	-2.605046000000	0.000000000000
B	0.000000000000	0.143523000000	0.000000000000
B	-1.466633000000	1.008414000000	0.000000000000
B	1.219214000000	-1.005899000000	0.000000000000
B	2.115458000000	-2.259993000000	0.000000000000
B	-0.541751000000	-1.558761000000	0.000000000000
C	-1.458012000000	-0.412996000000	0.000000000000
	10c		
Al	-0.732257000000	2.646160000000	0.000000000000
B	1.821166000000	-1.809107000000	0.000000000000
B	1.237904000000	-3.198144000000	0.000000000000
B	-1.518625000000	0.696166000000	0.000000000000
B	0.997465000000	-0.458540000000	0.000000000000
B	-0.772930000000	-0.730111000000	0.000000000000
B	0.138889000000	-2.127748000000	0.000000000000
C	0.000000000000	0.622889000000	0.000000000000

References

1. D. Sundholm, H. Fliegl and R. J. F. Berger, *Wiley Interdiscip. Rev. Comput. Mol. Sci*., 2016, **6**, 639–678.

2. J. Gauss and J. F. Stanton, *Electron-Correlated Approaches for the Calculation of NMR Chemical Shifts*. In: *Advances in Chemical Physics*. 2003, pp. 355–422.

3. P. Lazzeretti, *Prog. Nucl. Magn. Reson. Spectrosc*., 2000, **36**, 1–88.

4. D. Geuenich, K. Hess, F. Köhler and R. Herges, *Chem. Rev*., 2005, **105**, 3758–3772.

5. R. Herges and D. Geuenich, *J. Phys. Chem. A*., 2001, **105**, 3214–3220.