**SUPPLEMENTARY INFORMATION**

# $B_3Al_4^+$: A Three-Dimensional Molecular Reuleaux Triangle

Li-Xia Bai,[1] Mesias Orozco-Ic,[2,*] Ximena Zarate,[3] Dage Sundholm,[2] Sudip Pan,[4,*] Jin-Chang Guo,[1,*] and Gabriel Merino.[5,*]

[1] Nanocluster Laboratory Institute of Molecular Science Shanxi University, Taiyuan, 030006, China.

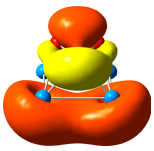
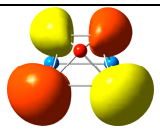
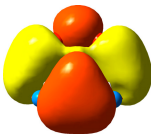
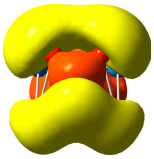
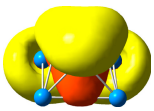
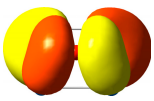
[2] Department of Chemistry, Faculty of Science, University of Helsinki, P.O. Box 55, A. I. Virtasen aukio 1, FIN-00014, Helsinki, Finland.

[3] Instituto de Ciencias Químicas Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Av. Pedro de Valdivia 425, Santiago, Chile.

[4] Fachbereich Chemie,Philipps-Universitt Marburg Hans-Meerwein-Straße,35043 Marburg, Germany.

[5] Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados, Unidad Mérida. Km 6 Antigua Carretera a Progreso. Apdo. Postal 73, Cordemex, 97310, Mérida, Yuc., México.

**Table S1.** Orbital composition analysis for occupied canonical molecular orbitals (CMOs) of $B_3Al_4^+$ global minimum ($C_s$, $^1A'$) cluster.

| CMO | $Al_4$ (%) | | $B_3$ (%) | |
|---|---|---|---|---|
| | s/p | total | s/p | total |
|  HOMO (a') | 35.9/31.1 | 67.0 | 9.2/21.3 | 30.5 |
|  HOMO−1 (a") | 51.0/19.8 | 70.8 | 15.2/12.1 | 27.3 |
|  HOMO−2 (a') | 0.9/43.8 | 44.7 | 2.6/50.4 | 53.0 |
|  HOMO−3 (a') | 7.8/25.8 | 33.7 | 19.3/44.6 | 63.9 |
|  HOMO−4 (a') | 35.0/11.4 | 46.4 | 4.6/46.2 | 50.9 |
|  HOMO−5 (a") | 39.7/9.3 | 49.0 | 0.0/49.0 | 49.0 |
|  HOMO−6 (a') | 28.4/6.6 | 35.0 | 16.3/45.2 | 61.5 |

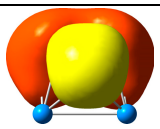
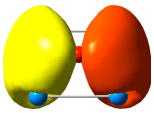
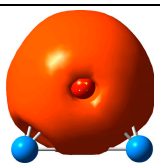
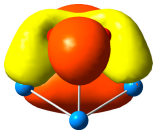
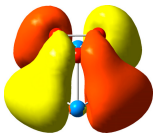
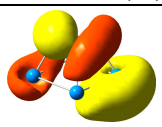
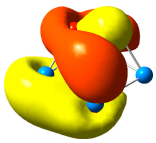
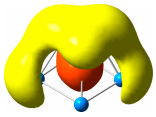
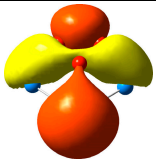
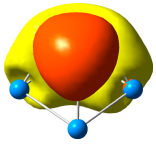
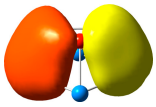
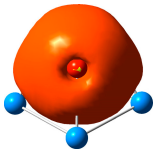
| | | | | |
|---|---|---|---|---|
|  HOMO−7 (a') | 37.4/8.5 | 45.9 | 11.0/39.5 | 50.4 |
|  HOMO−8 (a") | 25.7/7.2 | 33.0 | 21.9/41.7 | 63.6 |
|  HOMO−9 (a') | 7.8/5.8 | 13.6 | 52.7/28.8 | 81.5 |

**Table S2.** Orbital composition analysis for occupied canonical molecular orbitals (CMOs) of $B_3Al_4^+$ transition state ($C_s$, $^1A'$) cluster.

| CMO | $Al_4$ (%) | | $B_3$ (%) | |
|---|---|---|---|---|
| | s/p | total | s/p | total |
|  HOMO (a') | 45.7/23.8 | 69.6 | 11.5/16.7 | 28.2 |
|  HOMO–1 (a") | 3.9/49.5 | 53.4 | 6.5/37.8 | 44.3 |
|  HOMO–2 (a") | 37.3/21.3 | 58.7 | 9.2/30.2 | 39.4 |
|  HOMO–3 (a') | 24.0/29.4 | 53.4 | 12.7/31.4 | 44.1 |
|  HOMO–4 (a') | 20.9/7.6 | 28.5 | 10.9/57.8 | 68.6 |
|  HOMO–5 (a') | 38.3/9.9 | 48.2 | 0.2/49.6 | 49.8 |
|  HOMO–6 (a') | 30.9/6.8 | 37.8 | 11.8/46.7 | 58.5 |

| | | | | |
|---|---|---|---|---|
|  HOMO–7 (a") | 25.5/7.2 | 32.7 | 34.4/39.5 | 64.0 |
|  HOMO–8 (a') | 35.0/8.4 | 43.4 | 12.9/40.1 | 52.9 |
|  HOMO–9 (a') | 7.8/5.8 | 13.6 | 52.6/28.8 | 81.5 |

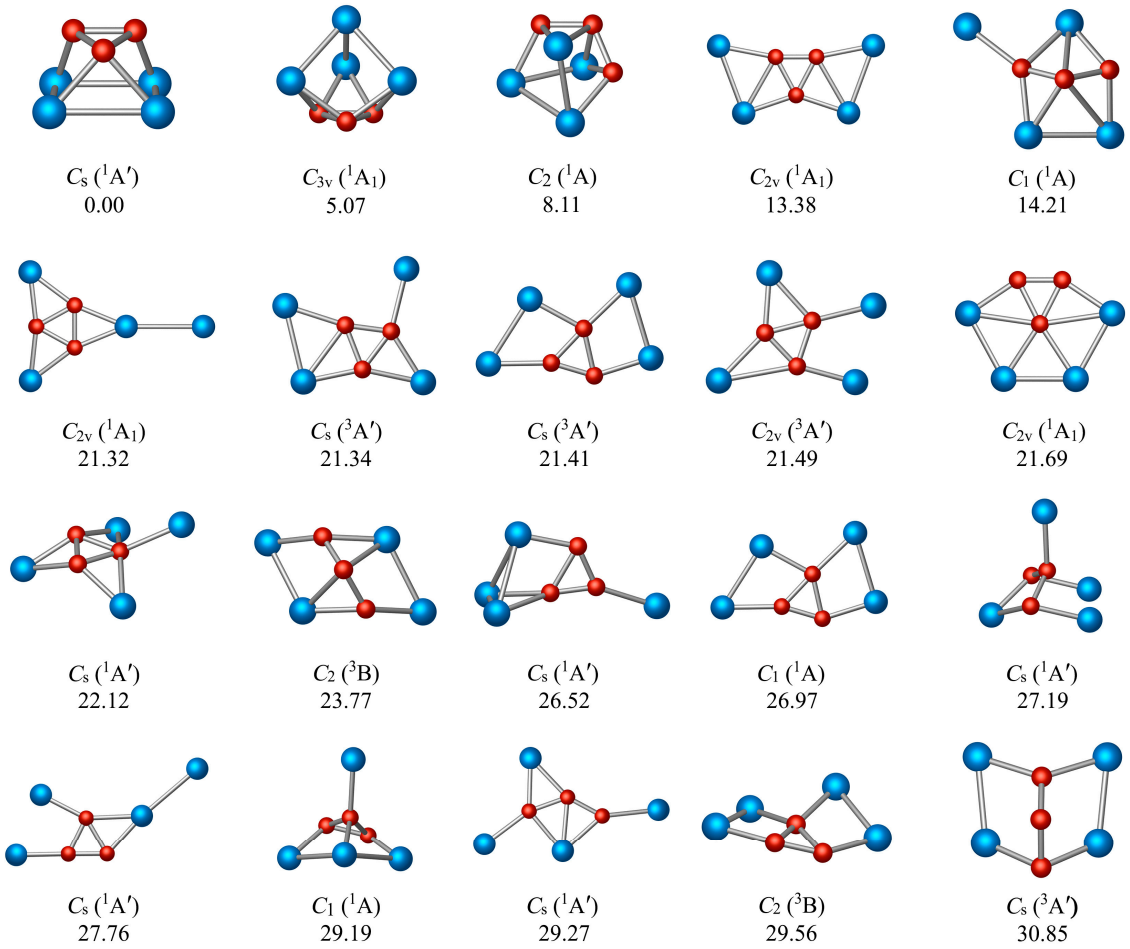



**Figure S1.** Twenty low-lying isomers of $B_3Al_4^+$. Relative energies are computed at the CCSD(T)/def2-TZVP//PBE0/def2-TZVP level (in kcal mol$^{-1}$).

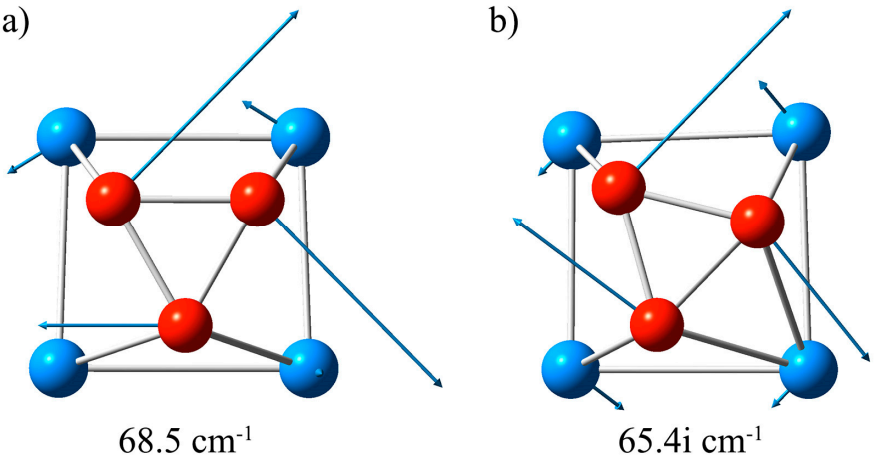



**Figure S2.** Displacement vectors of **a**) soft vibrational mode of the global minimum and **b**) the imaginary frequency of the transition state of $B_3Al_4^+$.

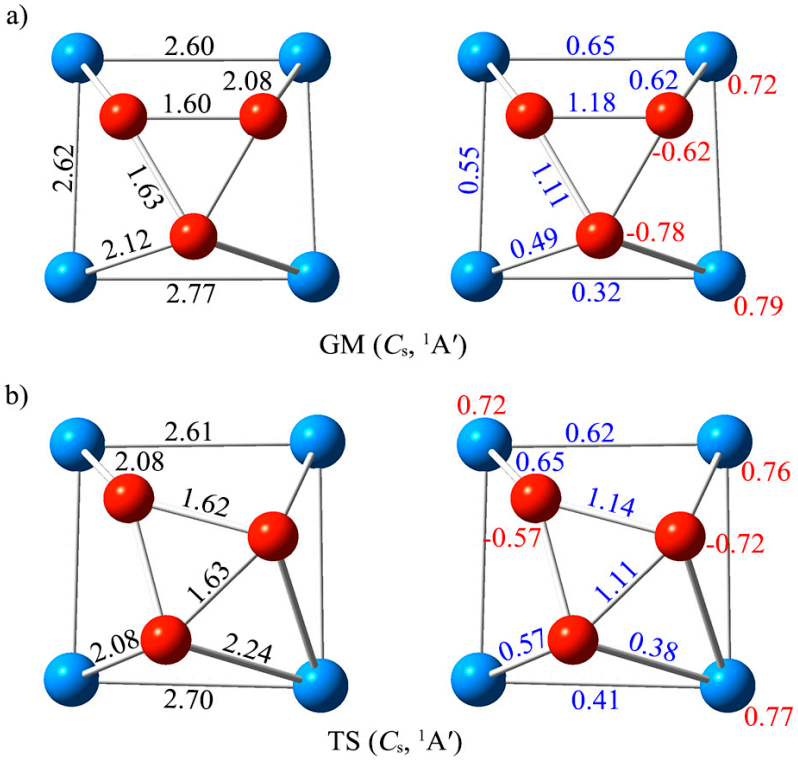



**Figure S3.** Computed bond distances (black color), Wiberg bond indices (WBIs; blue color) and natural atomic charges (in |e|; red color) for both the global minimum and the transition state structures of $B_3Al_4^+$.

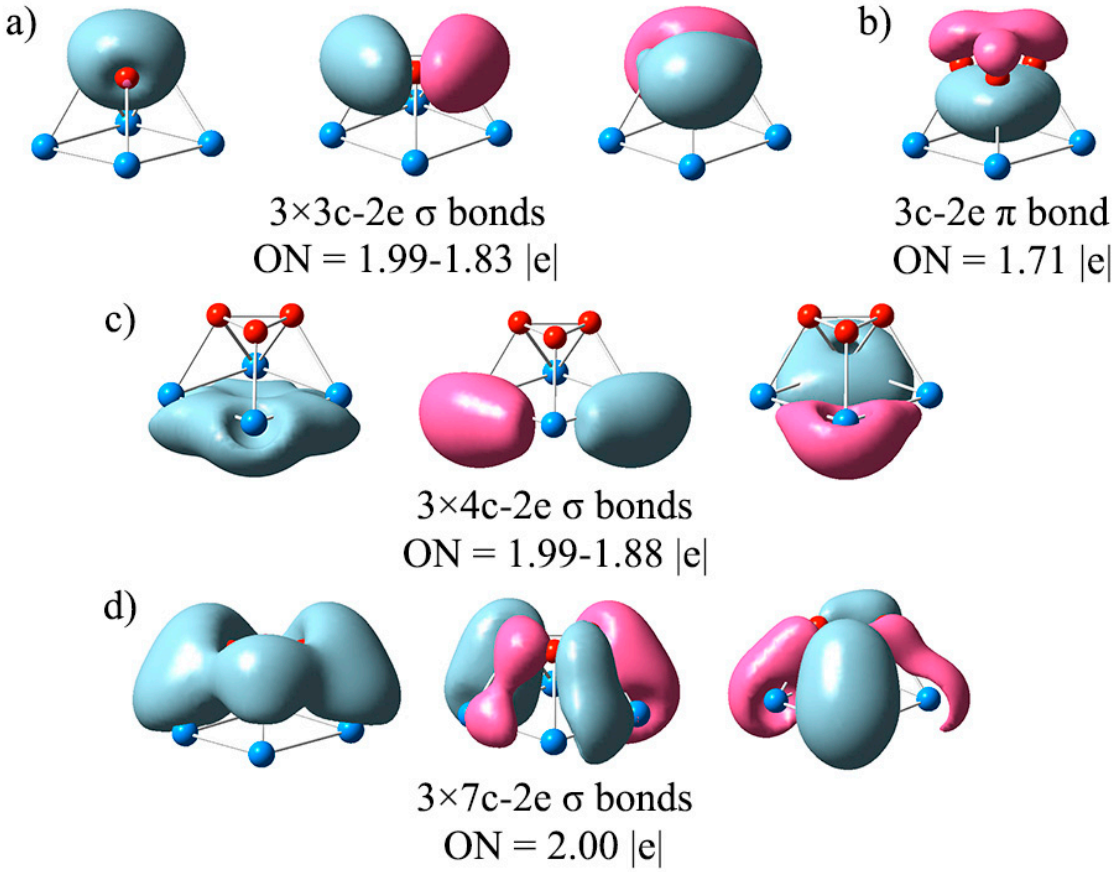



**Figure S4.** Bonding pattern, according to AdNDP analysis, in the transition state related to the rotation of the $B_3$ fragment in $B_3Al_4^+$. Occupation numbers (ONs) are shown.

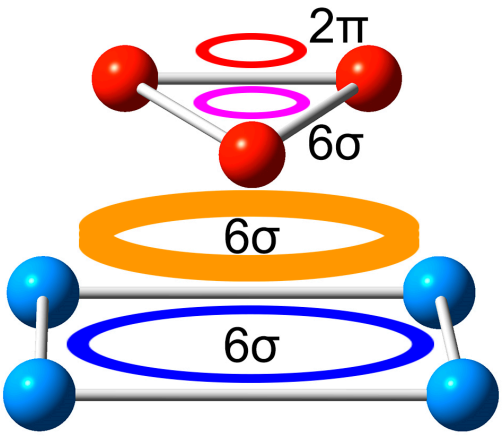



**Figure S5.** Bonding model for $B_3Al_4^+$.

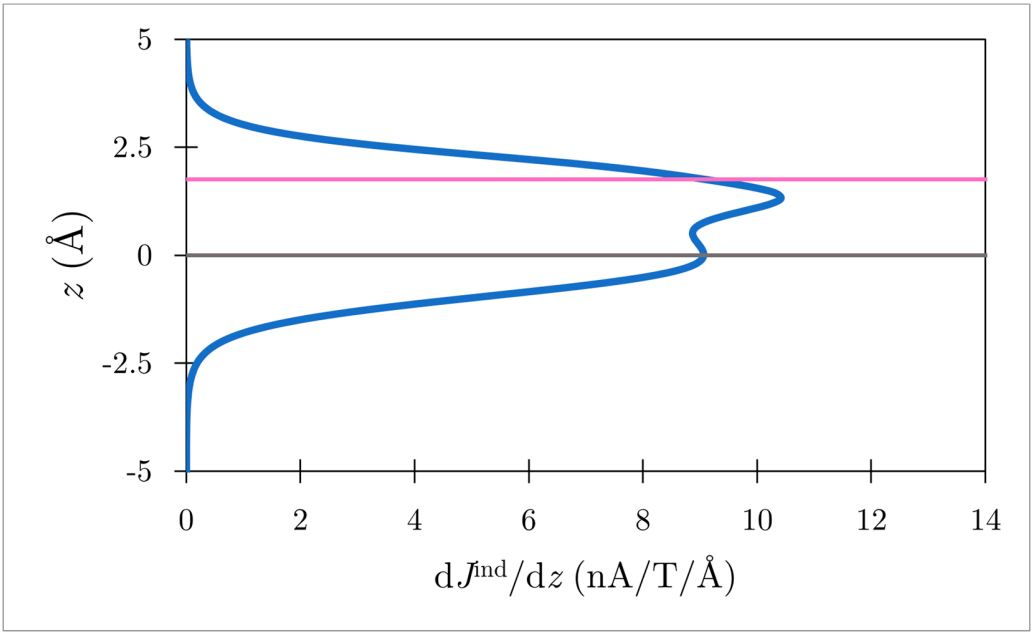



**Figure S6.** The vertical ring-current profile along the *z*-axis computed at the BHandHLYP/def2-TZVP level. The horizontal pink and gray lines correspond to the *z* values where the plane intersects the B-B and Al-Al bonds, respectively. Integrating the area under the d$J^{ind}$/d$z$ curve (in blue) yields the ring-current strength.

**Cartesian coordinates at the PBE0/def2-TZVP level**

**Global Minimum**

$B_3Al_4^+$

| | | | |
|---|---|---|---|
| Al | -1.25489400 | 0.63262100 | 1.30092700 |
| Al | 0.67957200 | -1.12963000 | 1.38492100 |
| Al | -1.25489400 | 0.63262100 | -1.30092700 |
| Al | 0.67957200 | -1.12963000 | -1.38492100 |
| B | 0.67957200 | 1.21159400 | 0.80231200 |
| B | 0.67957200 | 1.21159400 | -0.80231200 |
| B | 1.63252800 | 0.16125800 | 0.00000000 |

**Transition State**

$B_3Al_4^+$

| | | | |
|---|---|---|---|
| Al | -1.61037500 | -1.06640200 | 0.00000000 |
| Al | 0.07667300 | -0.38500100 | 1.85829700 |
| Al | 0.07667300 | -0.38500100 | -1.85829700 |
| Al | 1.87924500 | 0.37238500 | 0.00000000 |
| B | -1.25110800 | 0.97871600 | 0.00000000 |
| B | 0.07667300 | 1.41386700 | -0.81382900 |
| B | 0.07667300 | 1.41386700 | 0.81382900 |