

Supplementary Information

The scandium doped boron cluster $B_{27}Sc_2^+$: A fruit can-like structure

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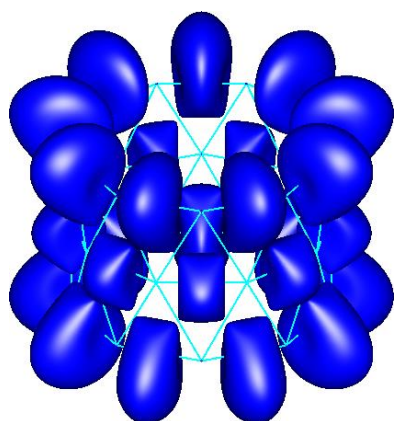
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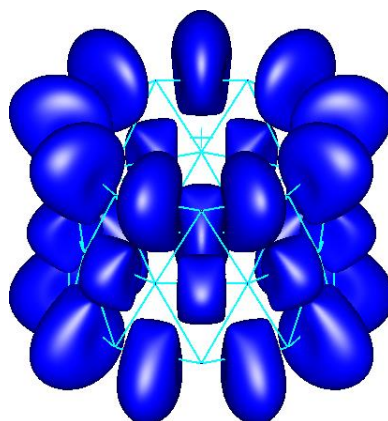
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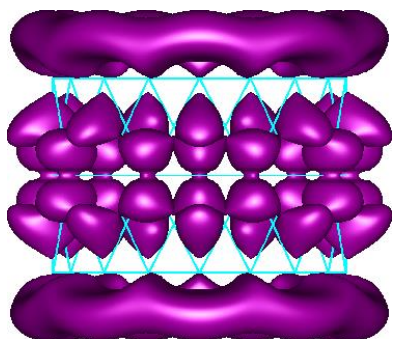
Email: minh.nguyen@kuleuven.be



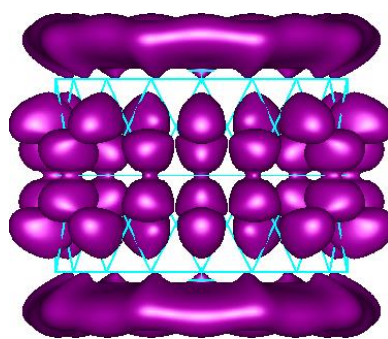
a) $ELF(\sigma_{loca}) = 0.81$



b) $ELF(\sigma_{loca}) = 0.81$



c) $ELF(\sigma_{delo}) = 0.90$



d) $ELF(\sigma_{delo}) = 0.89$

B_{27}^+ skeleton

$B_{27}Sc_2^+$

Figure S1. The $ELF(\sigma_{loca})$ maps for a) B_{27}^+ skeleton and b) the $B_{27}Sc_2^{2+}$ and the $ELF(\sigma_{delo})$ maps for c) B_{27}^+ skeleton and d) the $B_{27}Sc_2^{2+}$.

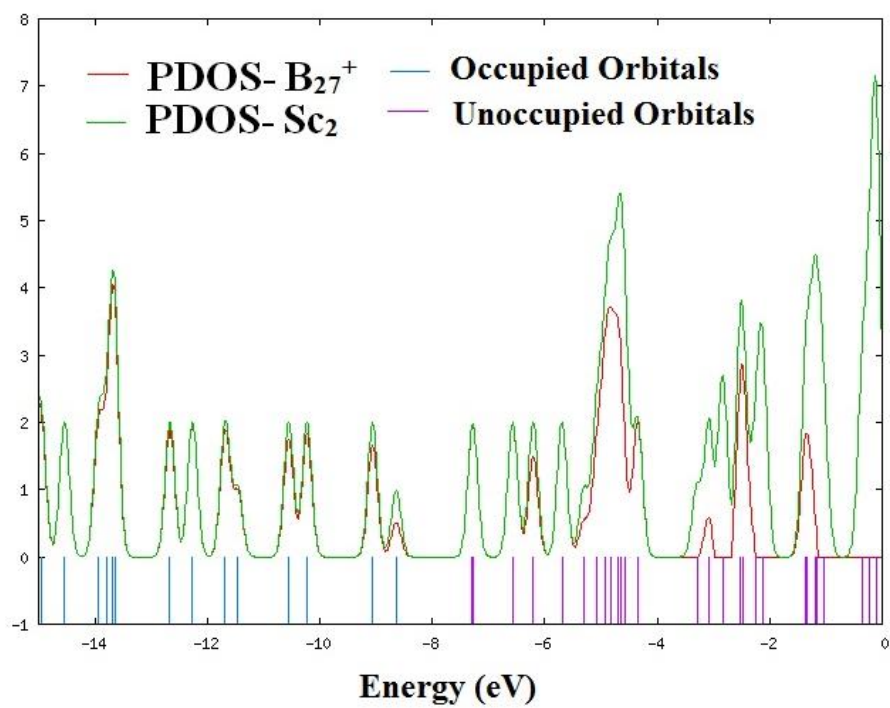
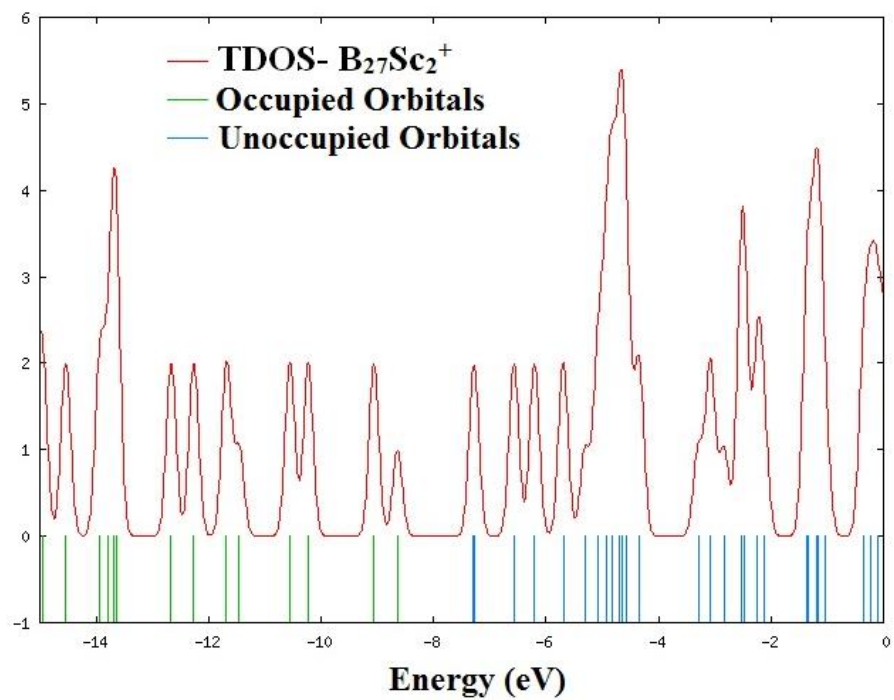
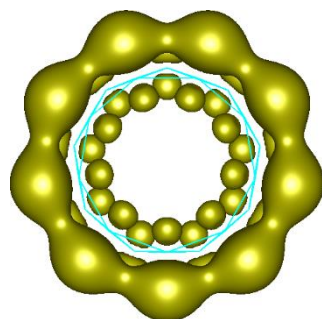
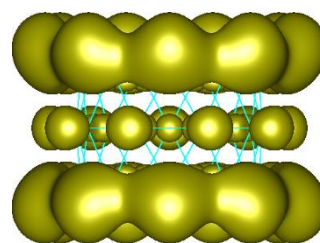


Figure S2. The DOS and PDOS spectra of the $B_{27}Sc_2^+$ obtained from TPSSh/def2-TZVP.

B_{27}^+ global

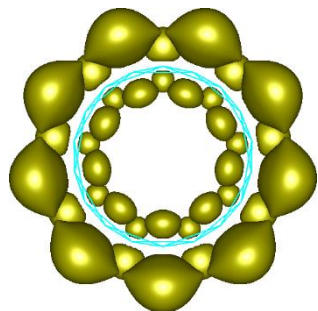


a)



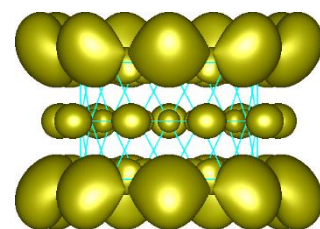
b)

B_{27}^+ skeleton



c)

Top view



d)

Side view

Figure S3. The ELF_{π} (isosurface = 0.81) maps for the B_{27}^+ global and B_{27}^+ skeleton under top view and side view.

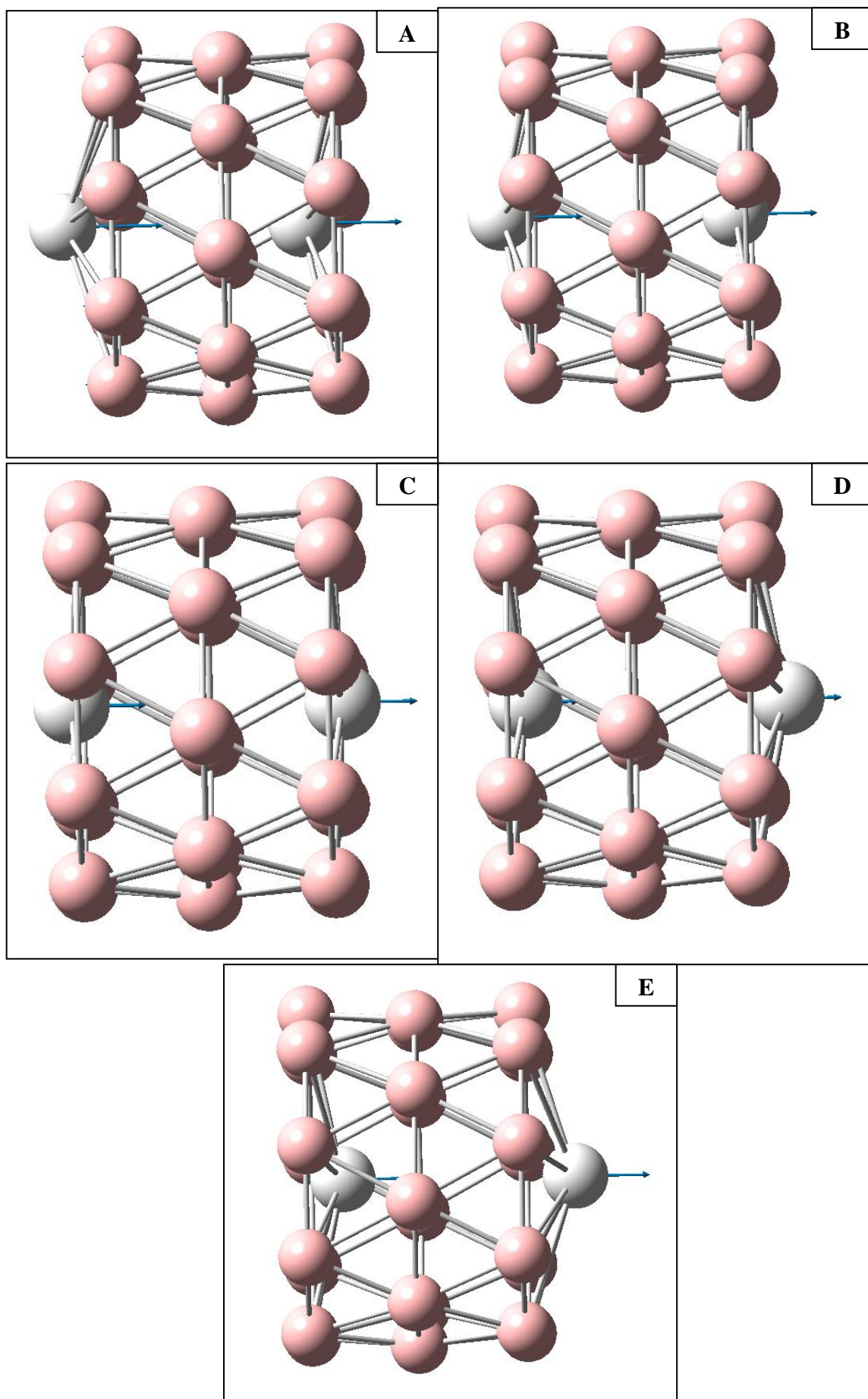


Figure S4. Frames of cation displacement at vibration frequency of 178 cm^{-1} .

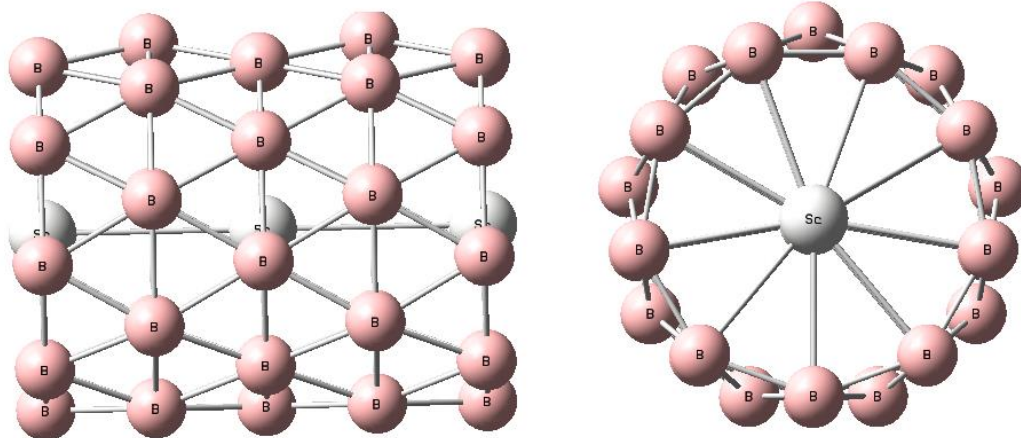


Figure S5. The relaxed geometries of $B_{45}Sc_3^+$ cation.

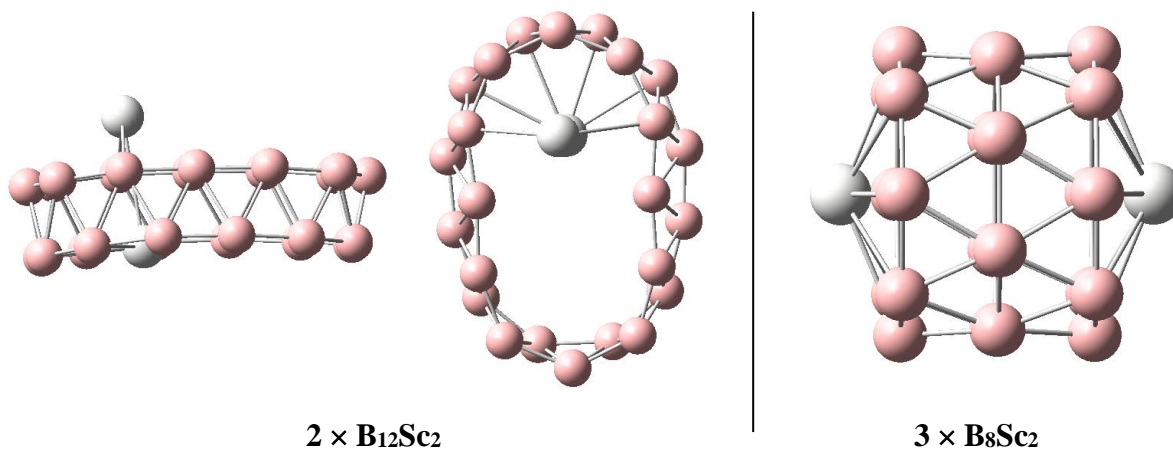


Figure S6. The relaxed geometries of $B_{24}Sc_2$.

Cartesian Coordinates of B₂₇Sc₂

B	2.071737000	-1.204204000	-1.547503000
B	-0.820508000	-2.254490000	1.493390000
B	0.820436000	-2.254531000	1.493387000
B	2.071567000	-1.207742000	1.544004000
B	2.368799000	0.391920000	1.518435000
B	1.535578000	1.812382000	1.519544000
B	0.000050000	2.361848000	1.526941000
B	-1.535507000	1.812431000	1.519548000
B	-2.368786000	0.392003000	1.518442000
B	-2.071609000	-1.207663000	1.544009000
B	0.820501000	-2.250864000	-1.498220000
B	2.368612000	0.395347000	-1.518092000
B	-0.000005000	-1.705468000	-0.001670000
B	1.673346000	-2.001013000	-0.002236000
B	2.509079000	-0.463044000	-0.000544000
B	2.032143000	1.139426000	0.000981000
B	0.861304000	2.341935000	0.002451000
B	-0.861184000	2.341896000	0.002453000
B	-2.032039000	1.139444000	0.000992000
B	-2.071791000	-1.204124000	-1.547490000
B	-0.820579000	-2.250822000	-1.498214000
B	-1.673364000	-2.000841000	-0.002233000
B	0.000043000	2.365289000	-1.521842000
B	1.535772000	1.816143000	-1.515830000
B	-1.535716000	1.816195000	-1.515821000
B	-2.368609000	0.395433000	-1.518083000
B	-2.509265000	-0.462967000	-0.000540000
Sc	0.000004000	-0.008652000	1.760249000
Sc	-0.000005000	-0.004186000	-1.759357000

Cartesian Coordinates of B₂₇Sc₂⁺

B	-2.388054000	-0.064505000	1.560046000
B	-0.351234000	-2.361625000	-1.560202000
B	-1.788460000	-1.584323000	-1.560545000
B	-2.388092000	-0.064537000	-1.559967000
B	-1.870370000	1.485315000	-1.560497000
B	-0.477943000	2.339824000	-1.560812000
B	1.138039000	2.099586000	-1.560464000
B	2.221706000	0.876883000	-1.560864000
B	2.266578000	-0.756401000	-1.561204000
B	1.249966000	-2.035849000	-1.560452000
B	-1.788393000	-1.584270000	1.560624000
B	-1.870306000	1.485333000	1.560523000
B	-1.149141000	-2.117564000	0.000027000
B	-2.246535000	-0.886661000	0.000039000
B	-2.284457000	0.761728000	0.000017000
B	-1.259625000	2.053301000	0.000001000
B	0.355343000	2.388640000	-0.000026000
B	1.799415000	1.594075000	-0.000047000
B	2.413994000	0.064272000	-0.000038000
B	1.250012000	-2.035811000	1.560458000
B	-0.351183000	-2.361586000	1.560250000
B	0.481566000	-2.354291000	0.000013000
B	1.138086000	2.099610000	1.560378000
B	-0.477896000	2.339865000	1.560782000
B	2.221772000	0.876925000	1.560767000
B	2.266621000	-0.756364000	1.561143000
B	1.890773000	-1.499709000	-0.000021000
Sc	-0.000293000	-0.000237000	-1.683177000
Sc	-0.000226000	-0.000206000	1.683194000