Electronic Supplementary Information

Binary mono-anions with unprecedented anti-aromatic planar tetracoordinate carbon and nitrogen atoms

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Contents

SI1: The results for the relative energies, the Iso-chemical shielding surfaces analysis, the NICSzz values of benzene, and the simulated PES spectra of **1**–**2.**

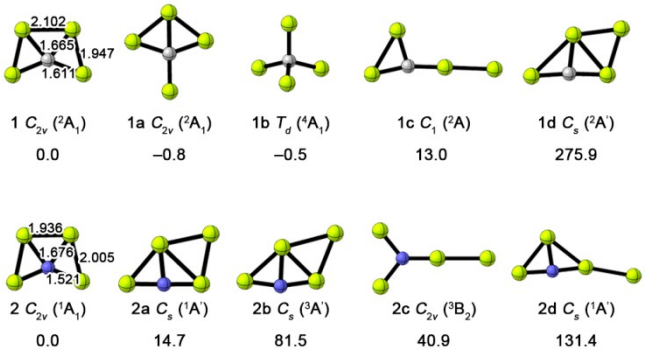

Fig. S1. The structures of CBe_4^- (**1**), NBe_4^- (**2**), and the concerned isomers. The relative energies (ΔE, in kcal mol^{-1}) are reported by considering multi-reference configuration interaction (MRCI).

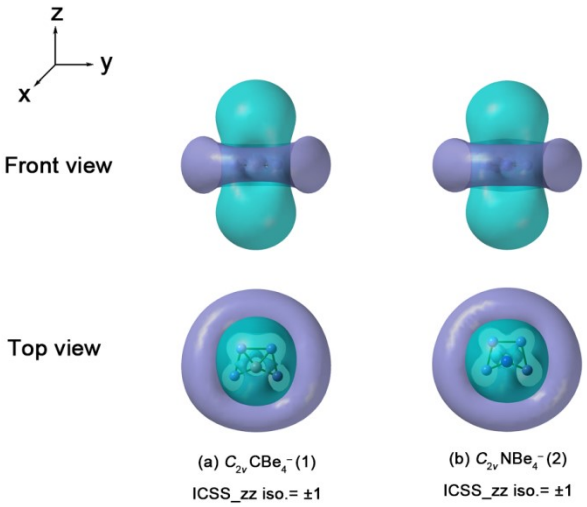

Fig. S2. Iso-chemical shielding surfaces (ICSSs, isovalue = ±1.0 ppm) of **1**–**2**. The chemical shielding and de-shielding areas are shown in purple and cyan, respectively.

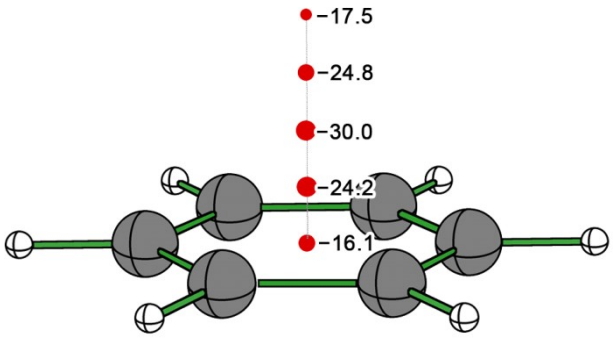

Fig. S3. The $NICS_{zz}$ values of benzene. Along the vertical line, the NICS points (green, red balls) are 0.5 Å apart from their neighbors.

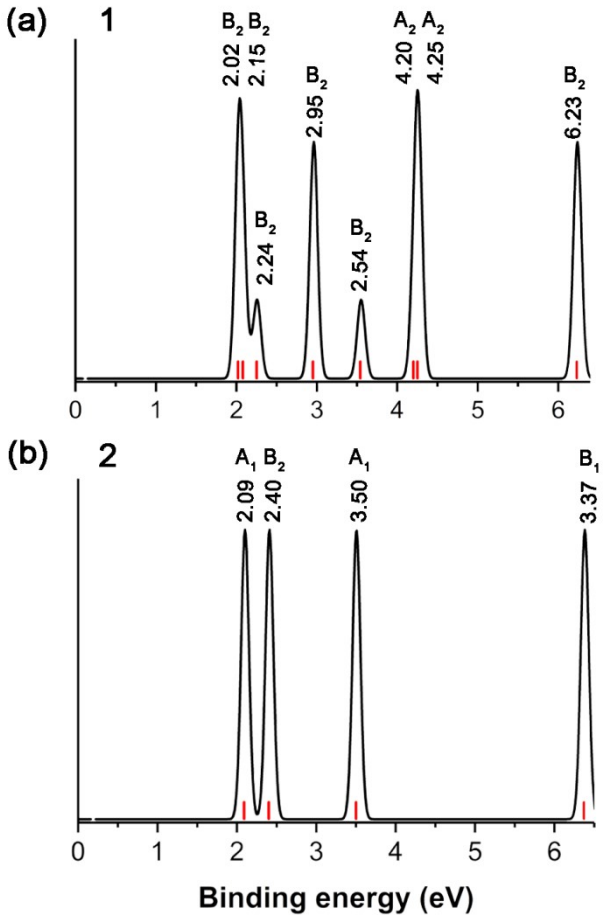

Fig. S4. Simulated PES spectra of CBe_4^- (**1**) and NBe_4^- (**2**) at the TD-B3LYP/aug-cc-pVTZ level, whose first VDEs were corrected using CCSD(T)/aug-cc-pVTZ calculations. The adsorption curves were simulated by fitting the calculated VDEs (vertical bars) using unit-area Gaussian function with half width of 0.1 eV.

SI2: Cartesian coordinates of B3LYP/aug-cc-pVTZ-optimized structures shown in Fig. 1

CBe_4^- (**1**)

C	0.00000000	0.00000000	0.24944900
Be	0.00000000	1.05095100	-1.04172300
Be	0.00000000	1.49284800	0.85463700
Be	0.00000000	-1.49284800	0.85463700
Be	0.00000000	-1.05095100	-1.04172300

1a

C	0.00000000	0.00000000	0.21950000
Be	0.00000000	1.52850800	-0.30671500
Be	0.00000000	-1.52850800	-0.30671500
Be	0.00000000	0.00000000	-1.51777300
Be	0.00000000	0.00000000	1.80195200

1b

C	0.00000000	0.00000000	0.00000000
Be	0.94469500	0.94469500	0.94469500
Be	-0.94469500	-0.94469500	0.94469500
Be	0.94469500	-0.94469500	-0.94469500
Be	-0.94469500	0.94469500	-0.94469500

1c

C	-0.57505900	-0.23553300	-0.00006500
Be	3.11638100	-0.03145000	-0.00369400
Be	-1.17019100	1.24086300	-0.00057700
Be	0.99829100	-0.14137100	0.00645300
Be	-2.08189300	-0.71474300	-0.00208400

1d

C	-0.65817300	0.35558400	0.00007000
Be	-2.11516800	-0.24943900	0.00021300
Be	0.75449200	1.10313000	-0.00026200
Be	2.12789300	-0.36881300	0.00038300
Be	0.22004200	-1.01825300	-0.00043800

NBe_4^- (**2**)

Be	1.41906600	0.84936900	-0.00008300
Be	0.97476200	-1.10364000	0.00007900
Be	-0.97476200	-1.10364000	0.00009900
Be	-1.41906600	0.84936900	-0.00005400
N	0.00000000	0.29059500	-0.00002300

2a

Be	1.35365200	1.33205800	0.00000000
Be	-1.35888000	0.04592300	0.00000000
Be	-0.82849400	-1.94700600	0.00000000
Be	0.83372300	-0.66887200	0.00000000
N	0.00000000	0.70737000	0.00000000

2b

N	0.00000000	0.83545000	0.00000000
Be	-1.19149500	-0.07229100	0.00000000
Be	-0.90550700	-2.17651200	0.00000000
Be	1.37651800	1.38158300	0.00000000
Be	0.72048400	-0.59481800	0.00000000

2c

N	0.00000000	0.00000000	0.56000500
Be	0.00000000	1.19293300	1.50448300
Be	0.00000000	-1.19293300	1.50448300
Be	0.00000000	0.00000000	-0.92690800
Be	0.00000000	0.00000000	-3.06206700

2d

N	0.00000000	0.64435500	0.00000000
Be	1.57372300	-2.64865000	0.00000000
Be	0.40081600	-0.80114600	0.00000000
Be	-0.48064100	2.05256200	0.00000000
Be	-1.49389800	0.26961300	0.00000000