Electronic Supplementary Information

Photoelectron Spectroscopy and Theoretical Study of Al_nC₅-^{/0} (n = 1-5) Clusters: Structural Evolution, Relative Stability of Star-Like Cluster and Planar Tetracoordinate Carbon Structure[†]

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Fig. S1. Photoelectron spectra of AlC_{14} clusters recorded with 266 nm photons.



Fig. S2. The low-lying isomers of anionic Al_5C_5 ⁻ clusters. The relative energies in the up line are calculated at the CCSD(T)/aug-cc-pVTZ level without taking into account ZPEs. In the down line are calculated at CCSD(T)/aug-cc-pVTZ/B3LYP/aug-cc-pVTZ level. Yellow and red balls stand for the Al and C atoms, respectively.



Fig. S3. Electron localization functions analysis of isomer 5a.



Fig. S4. The out-of-plane ZZ tensor component of iso-chemical shielding surfaces at 1 Å above the isomer 5a plane $[ICSS(1)_{zz}]$, calculated at B3LYP/6-311+G(d, p) level.