Supporting information for:

Comment on "Exploiting electronic strategies to stabilize a planar tetracoordinate carbon in cyclic aromatic hydrocarbons"

Venkatesan S. Thimmakondu*

Department of Chemistry and Biochemistry, San Diego State University, San Diego, CA 92182-1030, USA

E-mail: vthimmakondusamy@sdsu.edu

Table S1: Optimized geometries of the triplet ground electronic state ($\widetilde{X}^3\Sigma_g^-$) of heptatriynylidene (**1**) in Cartesian coordinates (in Ångström units) obtained at the UPBE0/def2-TZVP level of theory.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.293493
C	0.000000	0.000000	-1.293493
C	0.000000	0.000000	2.630584
C	0.000000	0.000000	-2.630584
C	0.000000	0.000000	3.882597
C	0.000000	0.000000	-3.882597
H	0.000000	0.000000	4.961512
H	0.000000	0.000000	-4.961512

Table S2: Optimized geometries of the singlet ground electronic state ($\widetilde{X}^1A'$) of 1-(buta-1,3-diynyl)cyclopropenylidene (**2**) in Cartesian coordinates (in Ångström units) obtained at the PBE0/def2-TZVP level of theory.

C	0.016996	1.573921	0.000000
C	0.000000	0.186267	0.000000
C	-0.040343	-1.056689	0.000000
C	-0.076715	-2.423979	0.000000
C	-0.109783	-3.656350	0.000000
H	-0.143307	-4.734900	0.000000
C	0.687644	2.764226	0.000000
C	-0.731571	2.857740	0.000000
H	1.665942	3.264084	0.000000

Table S3: Optimized geometries of the singlet ground electronic state ($\widetilde{X}^1A_1$) of $Si_2C_5H_2$ with a planar tetracoordinate carbon atom in Cartesian coordinates (in Ångström units) obtained at different levels.

CCSD/cc-pVDZ				CCSD/cc-pVTZ			
C	0.000000	0.000000	0.345625	C	0.000000	0.000000	0.341212
C	0.000000	-1.168284	-0.559120	C	0.000000	-1.159967	-0.557953
C	0.000000	1.168284	-0.559120	C	0.000000	1.159967	-0.557953
Si	0.000000	-1.808056	1.088963	Si	0.000000	-1.769091	1.081367
Si	0.000000	1.808056	1.088963	Si	0.000000	1.769091	1.081367
C	0.000000	-0.695706	-1.917122	C	0.000000	-0.689582	-1.900762
C	0.000000	0.695706	-1.917122	C	0.000000	0.689582	-1.900762
H	0.000000	-1.339007	-2.802742	H	0.000000	-1.323982	-2.774318
H	0.000000	1.339007	-2.802742	H	0.000000	1.323982	-2.774318