Theoretical Study of Si/C alternately substituted annulenes with a belt structure

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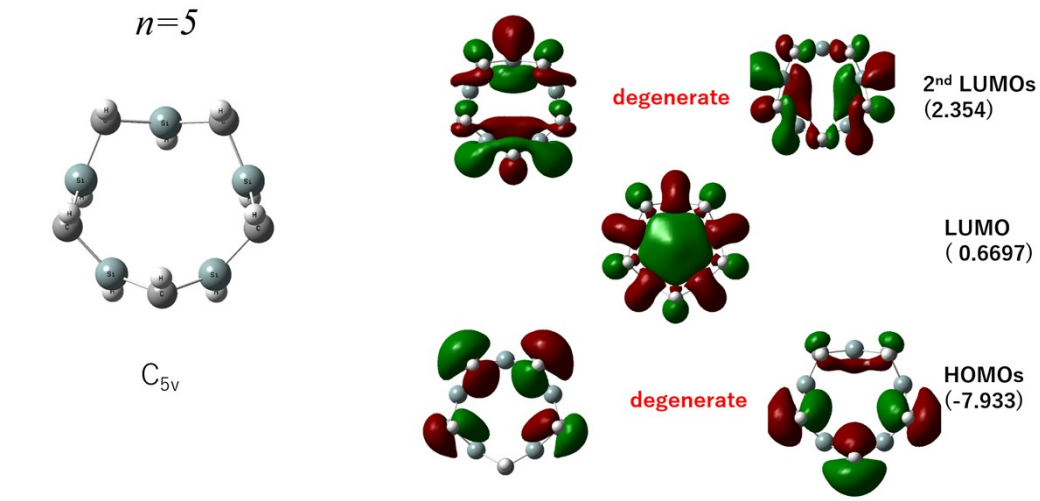
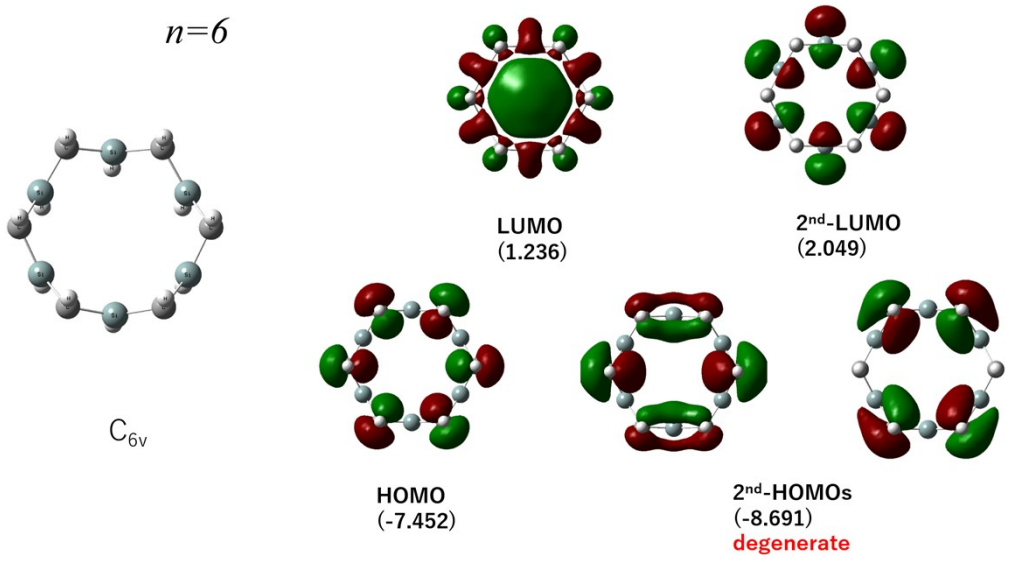
Supplementary Information

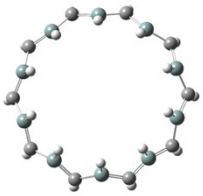
- Contents

Supplementary Figures

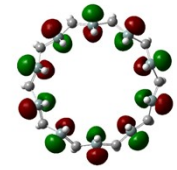




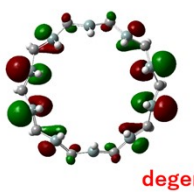
n=10

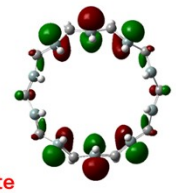


C_{10v}



LUMO
(1.398)

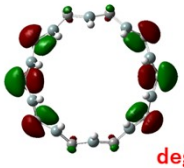




degenerate

2nd-LUMOs
(2.007)

HOMO
(-7.359)



degenerate

2nd-HOMOs
(-7.934)

$H_{20}C_{20}$

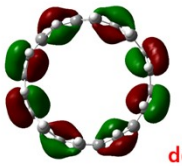
D_{10}

LUMO
(0.6319)

degenerate

2nd-LUMOs
(2.611)

HOMO
(-5.610)



degenerate

2nd-HOMOs
(-7.517)

Fig. SI1: The optimized structure and the frontier orbitals of the $H_{2n}Si_nC_n$ (n=5, 6,and10) and $H_{20}C_{20}$ belt type annulenes. For the molecular structure (left), light blue color shows Si atom, light gray color shows C atom, and white color does H. For the molecular orbitals, red color shows the plus orbital coefficients (isovalue=0.04) while green color does the minus ones. The numbers in parentheses are the orbital energies in eV.

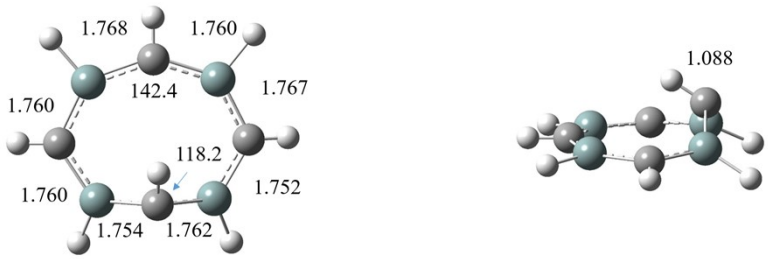


Fig. SI2: The optimized structure of iv on the potential energy surface of the isomerization of $H_8Si_4C_4$ (n=4) in Å and degrees (see Fig.7 in the main text). The left is the front view while the right is the side view.

Supplementary Tables

Table SI1: Weak (supporting) QUAO interactions of $H_6Si_3C_3$, $H_8Si_4C_4$, $H_{10}Si_5C_5$, $H_{12}Si_6C_6$, $H_{20}Si_{10}C_{10}$ isomers.

Interacting QUAOs	BO	KBO ($kcal/mol$)	Type of interaction
$H_6Si_3C_3$ – belt structure			
Siccπ – Siccπ	0.19	-1.90	weak conjugation
Csiσ – Siccπ	0.18	-1.37	hyperconjugation
Sicσ – Csisiπ	0.12	-1.36	hyperconjugation
Chσ – Sihσ	0.14	-1.22	σ conjugation
$H_6Si_3C_3$ – planar structure			
Si$^{c_i}\sigma$ – Si$^{c_i}\sigma$	0.07	-1.20	σ conjugation
Sihσ – Csiσ	0.13	-1.16	σ conjugation
Sicσ – Chσ	0.11	-1.01	σ conjugation
C$^{sisi\pi}$ – C$^{sisi\pi}$	0.14	-0.91	weak conjugation
$H_8Si_4C_4$ –belt structure			
Siccπ – Siccπ	0.27, 0.26	-3.23, -2.29	weak conjugation
C$^{sisi\pi}$ – C$^{sisi\pi}$	0.25	-1.38	weak conjugation
Chσ – Sihσ	0.13	-1.18	σ conjugation
Sicσ – Csiσ	0.14, 0.15	-0.72, -0.68	σ conjugation
$H_8Si_4C_4$ –planar structure			

$C^{sisi\pi}$ – $C^{sisi\pi}$	0.23	-1.98	weak conjugation
$Si^{c_i\sigma}$ – $Si^{c_i\sigma}$	0.07	-1.31	σ conjugation
Sic^{σ} – Ch^{σ}	0.12	-1.23	σ conjugation
Sih^{σ} – Csi^{σ}	0.12	-1.00	σ conjugation
$H_{10}Si_5C_5$ – belt structure			
$Sicc^{\pi}$ – $Sicc^{\pi}$		-1.91	weak conjugation
$C^{sisi\pi}$ – $C^{sisi\pi}$		-1.47	weak conjugation
Ch^{σ} – Sih^{σ}		-1.20	σ conjugation
Sic^{σ} – Csi^{σ}		-1.00	σ conjugation
Si_ic^{σ} – Si_ih^{σ}		0.80	σ conjugation
$H^{c_i\sigma}$ – Sic_i^{σ}		-0.70	σ conjugation
$Si^{c_i\sigma}$ – $Si^{c_i\sigma}$		-0.69	σ conjugation
$H_{12}Si_6C_6$ – belt structure			
$Sicc^{\pi}$ – $Sicc^{\pi}$		-1.80	weak conjugation
$C^{sisi\pi}$ – $C^{sisi\pi}$		-1.56	weak conjugation
Ch^{σ} – Sih^{σ}		-1.20	σ conjugation
Sic^{σ} – Csi^{σ}		-1.02	σ conjugation
$Si^{c_i\sigma}$ – $Si^{c_i\sigma}$		-0.99	σ conjugation
$H_{20}Si_{10}C_{10}$ – belt structure			
$C^{sisi\pi}$ – $C^{sisi\pi}$		-1.58	weak conjugation

$Si^{c_i\sigma}$ – $Si^{c_i\sigma}$		-1.21	σ conjugation
$Ch\sigma$ – $Sih\sigma$		-1.11	σ conjugation
$Sic\sigma$ – $Csi\sigma$		-1.08	σ conjugation
$Sicc\pi$ – $Sicc\pi$		-0.98	weak conjugation