Stereomutation in Tetracoordinate Centers via Stabilization of Planar Tetracoordinated Systems
Supporting Information

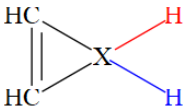
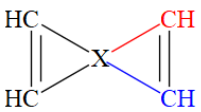
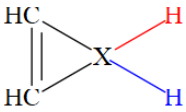
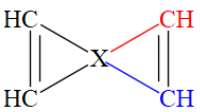
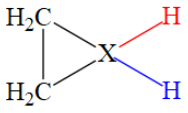
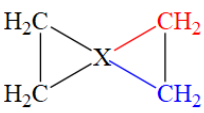
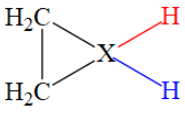
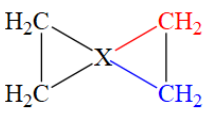
Komal Yadav [1], Upakarasamy Lourderaj [1,*] and U. Deva Priyakumar [2,*]

[1] *School of Chemical Sciences, National Institute of Science Education and Research, Bhubaneswar, HBNI, P.O. Jatani, Khordha, 752050, Odisha, India*
[2] *Center for Computational Natural Sciences and Bioinformatics International Institute of Information Technology, Hyderabad 500 032, India*

email: *u.lourderaj@niser.ac.in and deva@iiit.ac.in*

1 Relative Energies (including ZPE)

Table S1: Relative energies in kcal/mol including the zero-point energies of the neutral and dicationic species of cyclopropene, spiropentene, cyclopropane and spiropentane along with the skeletally substituted derivatives at the MP2/cc-pVTZ level of theory.

	Four valence electrons		Two valence electrons	
	$\Delta E_{\mathbf{ptX\text{-}ttX}}$		$\Delta E_{\mathbf{ptX\text{-}ttX}}$	
X				
B^-	76.2	42.3	-	−26.7
Al^-	27.9	12.6	−146.8	−7.9
Ga^-	38.3	17.6	−149.4	-
C	112.4	86.9	-	−19.1
Si	48.4	22.8	−8.7	−7.2
Ge	57.6	27.7	−8.5	−12.9
N^+	72.2	92.2	−4.5	−2.2
P^+	74.1	35.4	−63.4	−4.9
As^+	79.1	38.8	−78.5	−6.5
X				
B^-	146.1	98.5	−8.3	-
Al^-	41.4	29.2	−0.3	−13.5
Ga^-	55.9	42.7	−1.2	−23.4
C	106.5	99.0	-	−18.4
Si	75.0	57.1	−0.6	−9.7
Ge	82.2	67.2	−1.5	−15.8
N^+	66.9	62.8	-	-
P^+	72.2	99.1	−1.0	−3.2
As^+	62.9	105.0	−1.3	−8.4

2 Bond Index

The bond index for different heteroatom substituted molecules for cyclopropene, cyclopropane, spiropentene, and spiropentane were calculated using the natural bond orbital analysis. The Wiberg bond index for the X-C and C-C bonds for different systems are given below.

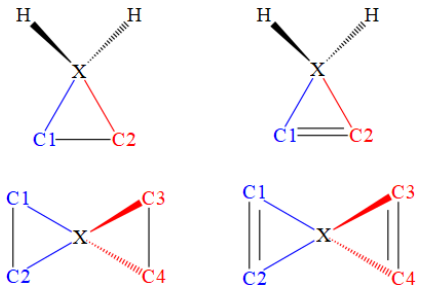


Figure S1: Representative structures for the calculation of bond indexes.

2.1 Cyclopropene derivatives

	Four valence electrons				Two valence electrons			
	ttX		**ptX**		**ttX**		**ptX**	
X	X-C1	C1-C2	X-C1	C1-C2	X-C1	C1-C2	X-C1	C1-C2
B^-	0.88	1.99	0.80	1.85	-	-	0.61	2.30
Al^-	0.62	2.04	0.54	1.97	0.48	1.03	0.18	2.80
Ga^-	0.68	2.06	0.56	1.97	0.62	1.03	0.20	2.77
C	0.99	1.97	0.44	2.45	-	-	1.03	1.74
Si	0.86	1.98	0.82	1.81	0.33	2.60	0.48	2.51
Ge	0.87	2.02	0.81	1.82	0.32	2.61	0.45	2.52
N^+	0.85	2.00	0.54	1.23	1.09	1.00	1.13	1.27
P^+	1.02	1.93	1.12	1.54	0.94	1.00	0.73	2.11
As^+	0.98	1.99	1.07	1.58	0.89	1.00	0.65	2.20

Table S2: Wiberg bond index for cyclopropene derivatives calculated for the geometries optimized at MP2/cc-pVTZ level of theory. '-' implies that the structures could not be optimized at the current level of theory.

2.2 Cyclopropane derivatives

	Four valence electrons				Two valence electrons			
	ttX		**ptX**		**ttX**		**ptX**	
X	X-C1	C1-C2	X-C1	C1-C2	X-C1	C1-C2	X-C1	C1-C2
B^-	0.88	1.00	0.86	1.12	0.37	1.64	0.45	1.59
Al^-	0.63	1.05	0.44	1.08	0.17	1.85	0.19	1.83
Ga^-	0.71	1.05	0.46	1.10	0.18	1.84	0.21	1.80
C	1.00	1.00	0.60	1.33	0.51	1.27	-	-
Si	0.85	1.04	0.63	1.06	0.37	1.58	0.39	1.55
Ge	0.89	1.05	0.26	1.76	0.37	1.58	0.39	1.55
N^+	0.87	1.03	0.57	1.19	-	-	0.59	1.00
P^+	0.98	1.04	0.44	1.48	0.43	1.15	0.45	1.16
As^+	0.96	1.06	0.43	1.51	0.45	1.20	0.47	1.20

Table S3: Wiberg bond index for cyclopropane derivatives calculated for the geometries optimized at MP2/cc-pVTZ level of theory. '-' implies that we were not able to locate the structures at the current level of theory.

2.3 Spiropentene derivatives

Four valence electrons								
	ttX				**ptX**			
X	X-C1	X-C3	C1-C2	C3-C4	X-C1	X-C3	C1-C2	C3-C4
B^-	0.86	0.86	1.93	1.93	0.81	0.81	1.87	1.87
Al^-	0.60	0.60	2.00	2.00	0.57	0.57	1.98	1.98
Ga^-	0.65	0.65	2.03	2.03	0.59	0.59	2.00	2.00
C	0.98	0.98	1.89	1.89	0.98	0.98	1.69	1.69
Si	0.83	0.83	1.92	1.92	0.80	0.80	1.86	1.86
Ge	0.84	0.84	1.97	1.97	0.79	0.79	1.90	1.90
N^+	0.87	0.87	1.92	1.92	0.69	0.69	2.07	2.07
P^+	0.99	0.99	1.84	1.84	0.99	0.99	1.71	1.71
As^+	0.97	0.97	1.91	1.91	0.95	0.95	1.77	1.77

Table S4: Wiberg bond index for spiropentene derivatives (X having four valence electrons) for the geometries optimized at MP2/cc-pVTZ level of theory.

Two valence electrons								
	ttX				**ptX**			
X	X-C1	X-C3	C1-C2	C3-C4	X-C1	X-C3	C1-C2	C3-C4
B^-	0.41	1.29	1.50	2.51	0.84	0.84	2.00	2.00
Al^-	0.60	0.86	0.22	1.86	0.60	0.60	2.25	2.25
Ga^-	-	-	-	-	0.65	0.65	2.21	2.21
C	0.52	1.46	2.23	1.23	0.96	0.96	1.77	1.77
Si	0.40	1.19	2.52	1.63	0.80	0.80	2.08	2.08
Ge	0.40	1.19	2.50	1.67	0.80	0.80	2.08	2.08
N^+	0.37	1.36	2.05	1.09	0.87	0.87	1.57	1.57
P^+	0.51	1.43	2.22	1.33	0.93	0.93	1.88	1.88
As^+	0.48	1.38	2.23	1.44	0.88	0.88	1.93	1.93

Table S5: Wiberg bond index for spiropentene derivatives (X having two valence electrons) for the geometries optimized at MP2/cc-pVTZ level of theory. '-' implies that we were not able to locate the structures at the current level of theory.

2.4 Spiropentane derivatives

Four valence electrons								
	ttX				**ptX**			
X	X-C1	X-C3	C1-C2	C3-C4	X-C1	X-C3	C1-C2	C3-C4
B^-	0.89	0.89	0.98	0.98	0.66	0.66	1.05	1.05
Al^-	0.60	0.60	1.04	1.04	0.50	0.50	1.06	1.06
Ga^-	0.69	0.69	1.04	1.04	0.50	0.50	1.05	1.05
C	0.99	0.99	0.98	0.98	0.78	0.78	1.12	1.12
Si	0.84	0.84	1.01	1.01	0.65	0.65	1.04	1.04
Ge	0.88	0.88	1.02	1.02	0.66	0.66	1.06	1.06
N^+	0.88	0.88	1.00	1.00	0.71	0.71	1.06	1.06
P^+	0.99	0.99	0.99	0.99	0.80	0.80	1.03	1.03
As^+	0.98	0.98	1.01	1.01	0.76	0.76	1.05	1.05

Table S6: Wiberg bond index for spiropentane derivatives (X having four valence electrons) for the geometries optimized at MP2/cc-pVTZ level of theory.

	Two valence electrons							
	ttX				**ptX**			
X	X-C1	X-C3	C1-C2	C3-C4	X-C1	X-C3	C1-C2	C3-C4
B^-	-	-	-	-	0.71	0.71	1.20	1.20
Al^-	0.21	0.78	1.80	1.01	0.56	0.56	1.30	1.30
Ga^-	0.24	0.85	1.76	1.11	0.60	0.60	1.26	1.26
C	0.47	1.17	1.29	0.91	0.81	0.81	1.12	1.12
Si	0.36	0.97	1.55	0.96	0.70	0.70	1.21	1.21
Ge	0.37	0.97	1.52	0.98	0.71	0.71	1.19	1.19
N^+	-	-	-	-	0.69	0.69	1.04	1.04
P^+	0.39	1.06	1.21	0.92	0.71	0.71	1.12	1.12
As^+	0.40	0.97	1.21	0.97	0.68	0.68	1.12	1.12

Table S7: Wiberg bond index for spiropentane derivatives (X having two valence electrons) for the geometries optimized at MP2/cc-pVTZ level of theory. '-' implies that we were not able to locate the structures at the current level of theory.

3 References

1. Wiberg, K. B. Application of the pople-santry-segal CNDO method to the cyclopropylcarbinyl and cyclobutyl cation and to bicyclobutane. *Tetrahedron*, **1968**, *24*, 1083-1096.