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Supplementary Material

Saturated N,X-Heterocyclic Carbenes (X = N, O, S, P, Si, C, and B): Stability, Nucleophilicity, and Basicity

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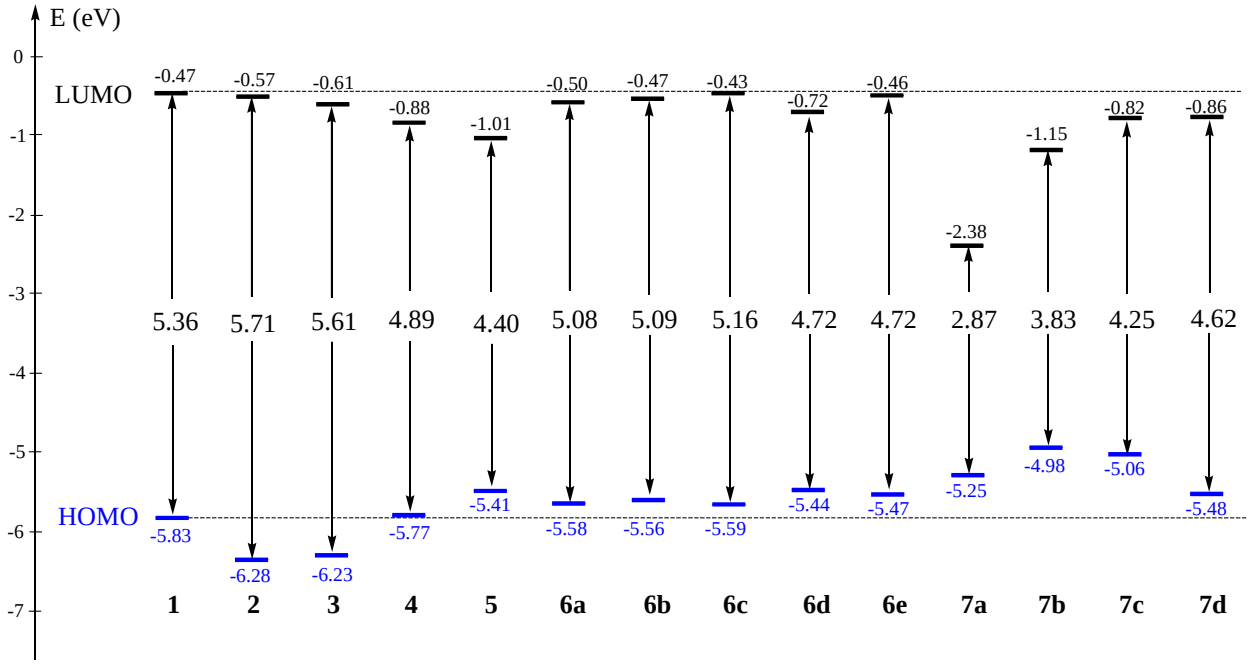


Figure S1. Graphical illustration of HOMO-LUMO gaps in the studied singlet carbenes at B3LYP/aug-cc-pVTZ.

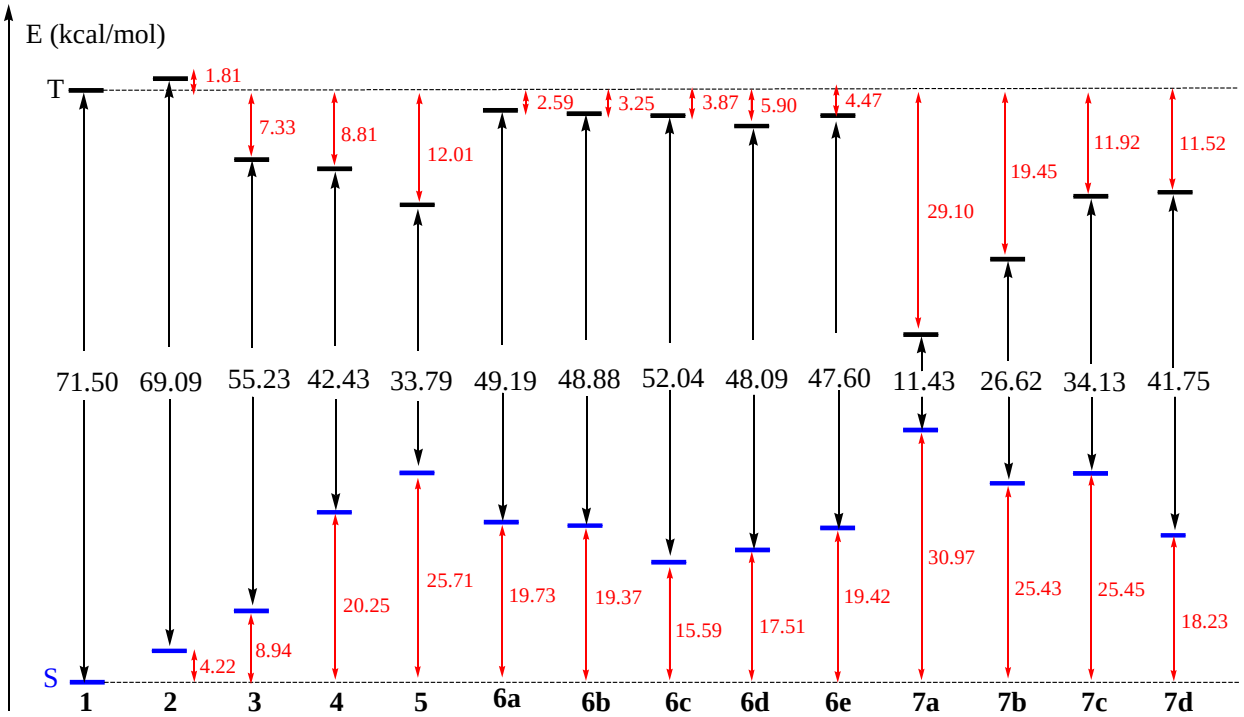


Figure S2. Graphical presentation of stabilizing and destabilizing energies of singlet and triplet states of the studied carbenes at B3LYP/aug-cc-pVTZ by isodesmic reactions

Isodesmic reactions

The isodesmic reaction rxn_1 shows that not only the singlet but also the triplet state is destabilized due to the presence of oxygen atom (Table 3 and Fig. S2). More specifically, the oxygen atom has a 4.22 kcal/mol destabilizing effect on the singlet state of carbene **2**(**s**) and 1.81 kcal/mol on the triplet state of carbene **2**(**t**); this indicates a slight decrease in the corresponding singlet–triplet energy gap in comparison with the ΔE_{s-t} value in carbene **1** (from 71.50 kcal/mol to 69.09 kcal/mol) as shown in Table 1. Reaction rxn_2 shows that the sulfur atom reduces the singlet–triplet energy gap to 55.23 kcal/mol (compared to ΔE_{s-t} = 71.50 kcal/mol for carbene **1**), due to an 8.94 kcal/mol destabilizing effect on the singlet-state **3**(**s**) and a 7.33 kcal/mol stabilizing effect on the triplet-state **3**(**t**), as illustrated in Table 1 and Fig. S2. Both oxygen and sulfur are π-donors; however, only oxygen has σ-acceptor property here, thus stabilizing the singlet state in carbene **2** more than in carbene **3**. The positive partial charge of sulfur atom along with the negative partial charge of the carbenic carbon (+0.24/–0.10 in Table 2) confirms that that sulfur atom has somewhat σ-donor characteristic, which destabilizes the singlet state of **3**.

An explanation similar to that expressed for oxygen and sulfur substitutions can justify the trends observed for destabilizing of the singlet state and stabilizing of the triplet state with the other substitutions. As such, the substituent groups of phosphorus (**4**) and silicon (**5**) have induced 20.25 and 25.71 kcal/mol destabilizing effects and 8.81 and 12.01 kcal/mol stabilizing effects on their corresponding singlet and triplet states, respectively. Carbene **4**, which possesses a phosphorus atom, has a moderate 42.43 kcal/mol singlet–triplet energy gap due to its π-donor/σ-donor property, while carbene **5** has a lower (33.79 kcal/mol) singlet–triplet energy gap because of a σ-donor power of its silicon atom. The spatial structure at phosphorus is not planar like nitrogen atom, and the orientation of its lone pair is not parallel to p_π orbital of the carbene [1]. Therefore, the π-donor character of P is weaker than of N atom, as also confirmed by their corresponding p_π(C:) values of 0.519 and 0.530, respectively (Table 2). Besides, phosphorus is even more electropositive than the carbenic carbon, conferring a σ-donor character to the phosphorous. As opposed to the σ-acceptor property of N, the σ-donor character of P destabilizes the carbene, hence reducing the stability of carbene **4** compared to carbene **1**. The silicon partial charge (q(Si) = 1.05) is more than the partial charge on phosphorus (q(P) = 0.47). When evaluated with the singlet–triplet energy gaps

of carbenes **4** and **5**, this indicates that the stability of carbene **5** is lower due to an additional σ-donor ability of Si compared to P atom. In addition, the lack of any π-donor feature in silicon also contributes to this result undoubtedly.

Contrary to nitrogen, carbon has no π-donation; this explains why the singlet states in series **6** are not as stabilized as that of carbene **1** (refer to the isodesmic reactions $rxn_{5–9}$). The singlet state of **6c** is destabilized less than those of other carbenes in the **6** series due to its saturated three-membered ring. The most viable justification for this higher stability seems to be the interaction of Walsh orbital with the carbenic p_π orbital (W→p_π), as illustrated in Fig. 2. This interaction lowers the energy level of the singlet state in **6c** in comparison with other carbenes in series **6**. The HOMO-3 molecular orbital depicts this effect well (Fig. 2). According to the isodesmic reaction rxn_9, the six-membered ring (in **6e**) can induce a smaller effect on the singlet-state stability of the carbene with respect to the three-membered ring (in **6c**).

In general, the isodesmic reactions rxn_{10} and rxn_{11} prove that the singlet and triplet states of carbenes **7** are destabilized and stabilized compared to those in carbene **1**, respectively. In **7a**, the boron adjacent to the carbenic center has the most destabilizing effect on the singlet state (30.97 kcal/mol) and the most stabilizing effect on the triplet state (29.10 kcal/mol) because of its σ-donor/π-acceptor property. The higher partial positive charge on boron atom (q(B) = 2.00) points to a stronger σ-donor character of **7a** compared to all other carbenes studied here (Table 2). Compared to **7a**, the addition of NH_2 to boron atom in carbene **7b** has increased its singlet–triplet energy gap from 11.43 to 26.62 kcal/mol. The amino group is able to donate electrons into the vacant p orbital of its neighboring boron atom, thus increasing the electron density on the boron. Consequently, the presence of the amino group not only decreases the stabilization effect on the triplet state of **7b**, but also reduces the σ-donation character of boron atom (q(B) = 0.67 and q(C:) = –0.18), which altogether lead to a higher stability of its corresponding singlet state.

Reference:

[1] M. Rullich, R. Tonner, G. Frenking, P-Heterocyclic carbenes as effective catalysts for the activation of single and multiple bonds. A theoretical study, New Journal of Chemistry 34 (2010) 1760–1773.

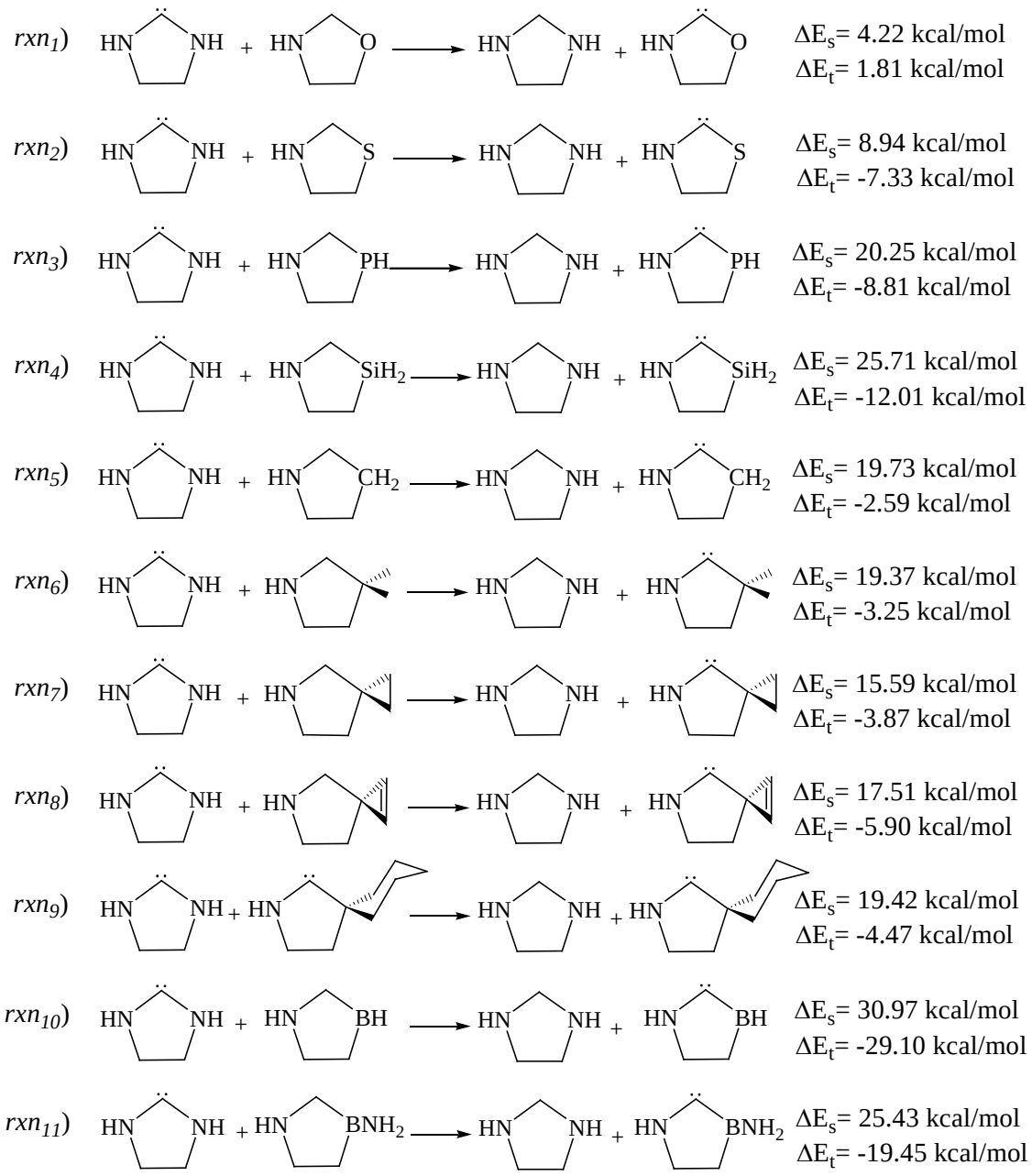


Figure S3. The extended isodesmic reactions *rxn*$_{1-11}$, for singlet (ΔE_s) and triplet states (ΔE_t) in kcal/mol at B3LYP/aug-cc-pVTZ

Table S1. Smallest vibrational frequencies υ_{min} (cm^{-1}) for the studied species at the B3LYP/6-31+G* level.

Struct.	υ_{min}	Struct.	υ_{min}	Struct.	υ_{min}	Struct.	υ_{min}	Struct.	υ_{min}
1(s)	126.7218	**1(t)**	107.5328	**1-H$_2$**	66.5081	**1-d**	26.7496	**1-d**	—
2(s)	64.8574	**2(t)**	93.9948	**2-H$_2$**	86.4777	**2-d-E**	50.3507	**2-d-Z**	35.4139
3(s)	110.2481	**3(t)**	142.8504	**3-H$_2$**	127.3693	**3-d-E**	49.0286	**3-d-Z**	40.4931
4(s)	125.7046	**4(t)**	125.6741	**4-H$_2$**	128.0814	**4-d-E**	57.9398	**4-d-Z**	26.5458
5(s)	40.6581	**5(t)**	134.7786	**5-H$_2$**	125.2709	**5-d-E**	52.9696	**5-d-Z**	41.9522
6a(s)	125.7087	**6a(t)**	63.1351	**6a-H$_2$**	86.8698	**6a-d-E**	45.9318	**6a-d-Z**	41.6744
6b(s)	102.0181	**6b(t)**	46.0437	**6b-H$_2$**	46.7345	**6b-d-E**	50.7299	**6b-d-Z**	43.8759
6c(s)	61.6392	**6c(t)**	77.8922	**6c-H$_2$**	48.4529	**6c-d-E**	15.4611	**6c-d-Z**	42.1213
6d(s)	41.8931	**6d(t)**	115.4940	**6d-H$_2$**	58.3095	**6d-d-E**	35.9331	**6d-d-Z**	47.9934
6e(s)	81.2947	**6e(t)**	54.0646	**6e-H$_2$**	57.4144	**6e-d-E**	—	**6e-d-Z**	—
7a(s)	96.6719	**7a(t)**	118.5180	**7a-H$_2$**	211.8770	**7a-d-E**	59.9934	**7a-d-Z**	76.7049
7b(s)	67.5005	**7b(t)**	146.7815	**7b-H$_2$**	107.8869	**7b-d-E**	59.6988	**7b-d-Z**	68.4765

Table S2. The $<S^2>$ values for the investigated triplet state carbenes at different level of theory

Struct.	U-CCSD(T)/6-311+G** S^2	U-QCISD/6-31G* S^2	U-B3LYP/6-31+G* S^2
1t	2.01481	2.01298	2.00636
2t	2.01273	2.00268	2.00558
3t	2.01958	2.01722	2.00820
4t	2.02309	2.02106	2.00784
5t	2.01966	2.01788	2.00723
6a-t	2.01610	2.01422	2.00608
6b-t	2.01590	2.01405	2.00606
6c-t	2.01882	2.01694	2.00654
6d-t	2.02236	2.02510	2.00829
6e-t	2.01598	2.01417	2.00578
7a-t	2.01352	2.01103	2.00465
7b-t	2.01665	2.01434	2.00604

Table S3. The absolute energies (Hartree) and zero point vibrational energy (ZPVE, in kcal/mol) for the investigated singlet and triplet states carbenes.

Structure	B3LYP/6-31+G* ZPVE (kcal/mol)	B3LYP/aug-cc-pVTZ HF
1s	59.10164	-227.468413
1t	57.80602	-227.3544683
2s	51.03186	-247.3351985
2t	50.14275	-247.2250887
3s	49.31953	-570.3134492
3t	48.53071	-570.2254259
4s	54.68339	-514.0548665
4t	53.5746	-513.9872467
5s	59.01844	-462.7942853
5t	58.42783	-462.7404433
6a-s	66.19817	-211.4002987
6a-t	65.14397	-211.3219137
6b-s	101.45137	-290.0574519
6b-t	100.36262	-289.9795583
6c-s	87.53665	-288.8165275
6c-t	86.34156	-288.7335977
6d-s	71.37606	-287.5406708
6d-t	70.26275	-287.4640338
6e-s	143.18124	-406.8299032
6e-t	142.10508	-406.754041
7a-s	55.48614	-197.5094243
7a-t	55.28855	-197.49121
7b-s	68.13761	-252.9645111
7b-t	67.2511	-252.9220912

Table S4. The T1 diagnostic values for the studied species at CCSD(T)/6-311+G** level

Structure	T1	Structure	T1
1s	0.01540415	**6a-t**	0.01465997
1t	0.01616395	**6b-s**	0.01362179
2s	0.01688427	**6b-t**	0.01378964
2t	0.01665855	**6c-s**	0.0137908
3s	0.01715741	**6c-t**	0.01414008
3t	0.0193631	**6d-s**	0.01454869
4s	0.01681155	**6d-t**	0.01640097
4t	0.01756207	**7a-s**	0.0179152
5s	0.01653736	**7a-t**	0.02291285
5t	0.01726339	**7b-s**	0.01687298
6a-s	0.01502881	**7b-t**	0.01934476

Table S5. Topological parameters of the bond critical point (BCP) at the B3LYP/6-311+G*// B3LYP/6-31+G* level.

Structure	[a]BCP	R	[b] ρ_b (a.u.)	λ_1 (a.u.)	λ_2 (a.u.)	λ_3 (a.u.)	[c] $\nabla^2\rho_b$ (a.u.)	ε
1	N-C:	1.351	0.316	-0.694	-0.601	0.553	-0.742	0.154
2	N-C:	1.337	0.327	-0.726	-0.681	0.617	-0.790	0.066
3	N-C:	1.324	0.328	-0.722	-0.617	0.710	-0.629	0.170
4	N-C:	1.313	0.329	-0.751	-0.584	0.868	-0.467	0.285
5	N-C:	1.307	0.328	-0.757	-0.530	0.984	-0.303	0.427
6a	N-C:	1.315	0.331	-0.770	-0.602	0.879	-0.493	0.280
6b	N-C:	1.313	0.332	-0.774	-0.609	0.895	-0.489	0.271
6c	N-C:	1.319	0.328	-0.758	-0.594	0.841	-0.511	0.276
6d	N-C:	1.317	0.329	-0.766	-0.594	0.877	-0.483	0.290
6e	N-C:	1.312	0.332	-0.774	-0.607	0.900	-0.481	0.277
7a	N-C:	1.314	0.323	-0.756	-0.505	0.992	-0.269	0.497
7b	N-C:	1.312	0.325	-0.765	-0.512	0.991	-0.286	0.492
CH_3─NH_2	N-C		0.258	-0.504	-0.486	0.347	-0.642	0.036
Pyridine	N-C		0.338	-0.723	-0.655	0.399	-0.979	0.104
DBN	N-C		0.381	-0.885	-0.704	0.500	-1.088	0.257

[a] BCP: Bond Critical Point
[b] The electron density at the BCP
[c] The Laplacian of the electron density at the BCP, $\nabla^2\rho_b = \lambda_1 + \lambda_2 + \lambda_3$, λ_i is an eigenvalue of the Hessian matrix of ρ_b

Table S6. Topological parameters of the bond critical point (BCP) at the B3LYP/6-311+G*// B3LYP/6-31+G* level.

Structure	[a]BCP	R	[b] ρ_b (a.u.)	λ_1 (a.u.)	λ_2 (a.u.)	λ_3 (a.u.)	[c] $\nabla^2\rho_b$ (a.u.)	ε
2	O-C:	1.339	0.294	-0.710	-0.530	1.054	-0.186	0.341
3	S-C:	1.732	0.211	-0.329	-0.299	0.245	-0.383	0.100
4	P-C:	1.845	0.162	-0.204	-0.178	0.316	-0.066	0.142
5	Si-C:	1.907	0.120	-0.160	-0.153	0.487	0.174	0.042
6a	C-C:	1.520	0.251	-0.483	-0.468	0.371	-0.579	0.033
6b	C-C:	1.533	0.249	-0.481	-0.461	0.374	-0.568	0.044
6c	C-C:	1.488	0.267	-0.514	-0.509	0.368	-0.655	0.011
6d	C-C:	1.497	0.264	-0.509	-0.505	0.374	-0.640	0.007
6e	C-C:	1.534	0.248	-0.478	-0.458	0.373	-0.564	0.044
7a	B-C:	1.612	0.182	-0.373	-0.283	0.297	-0.359	0.315
7b	B-C:	1.602	0.183	-0.355	-0.302	0.344	-0.313	0.178

[a] BCP: Bond Critical Point

[b] The electron density at the BCP

[c] The Laplacian of the electron density at the BCP, $\nabla^2\rho_b = \lambda_1 + \lambda_2 + \lambda_3$, λ_i is an eigenvalue of the Hessian matrix of ρ_b

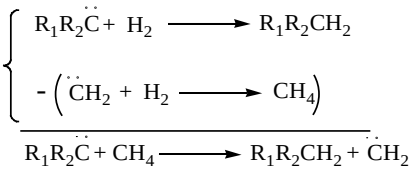
Carbene Stabilization Enthalpies (CSE)

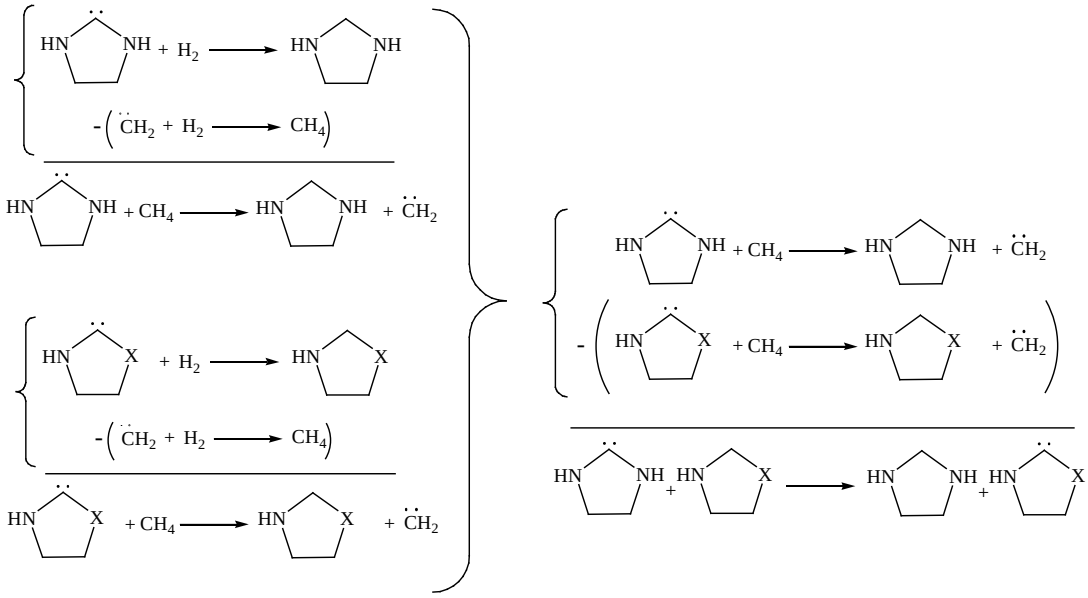
To make easy comparisons, Scott Gronert et al. reported the carbene stabilization enthalpies (CSEs), measured as the difference in heat of hydrogenation of a carbene (CR_1R_2) from the corresponding value for the parent methylene as shown in Eq. (1) [1]. The values of CSE represent substituent effects (of R_1 and R_2) on stabilities of carbenes, with the unsubstituted (singlet or triplet) methylene taken as reference.

$$\text{CSE } (R_1R_2) = \Delta H_{\text{Hydrogenation}}(CR_1R_2) - \Delta H_{\text{Hydrogenation}}(CH_2) \quad (1)$$

In this work, to reach a clear overview of different substituent effects on singlet and triplet states, we designed a set of efficient isodesmic reactions. Indeed, the isodesmic reactions employed based on all the equations below in this work are exactly equal with the Gronert method (CSE).

CSE based on isodesmic reaction





[1] Gronert, S.; Keeffe, J. R.; O'Ferrall, R. A. M. Stabilities of Carbenes: Independent Measures for Singlets and Triplets. *J. Am. Chem. Soc.*, **2011**, *133*, 3381–3389.

Cartesian coordinates for all calculated structures (B3LYP/6-31+G*)

1(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.76792700	0.93257700	-0.08037000
C	-0.00141200	-1.33501900	-0.00000400
C	-0.76599000	0.93399300	0.08029600
H	1.07572200	1.28406300	-1.07447500
H	1.27461500	1.53736800	0.67770800
H	-1.27180800	1.53984600	-0.67754400
H	-1.07265500	1.28632700	1.07450600
N	-1.06506200	-0.50648200	-0.08333800
H	-2.00627000	-0.86379300	-0.01998200
N	1.06402600	-0.50856700	0.08341200
H	2.00449600	-0.86777700	0.01973800

1(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.78452600	0.85579700	-0.17473300
C	-0.00728800	-1.22765600	-0.21152600
C	0.74164400	0.91629600	0.12604200
H	-1.37094200	1.55625400	0.42762600
H	-0.97415700	1.05286200	-1.23432600
H	0.93072300	1.21635100	1.16608400
H	1.26669800	1.61017300	-0.53908700
N	1.18745200	-0.48710500	-0.10824100
H	1.86705200	-0.82081100	0.57640700
N	-1.17994600	-0.54562300	0.11773600
H	-1.47090100	-0.65234700	1.09813300

2(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	1.04824100	0.57078100	0.00005500
C	-0.44640700	-1.24119200	0.00000700
C	-0.37177600	1.15064700	-0.00005300
H	1.62512300	0.81930400	-0.89305400
H	1.62492800	0.81919900	0.89332200
H	-0.59074900	1.74854600	-0.89109300
H	-0.59079700	1.74872500	0.89085400
N	-1.15206600	-0.10571200	0.00004900
H	-2.16210400	-0.12250700	0.00001600
O	0.84721500	-0.89433700	-0.00005500

2(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.86213400	0.79367800	0.10662000
C	0.11794100	-1.20132800	-0.22558000
C	0.66242900	0.94606500	-0.16420400
H	-1.15773000	1.11866600	1.10959800
H	-1.48293000	1.29499800	-0.64143100
H	1.14299800	1.68606200	0.48248500
H	0.85066400	1.20830800	-1.20921400
N	1.21179000	-0.41057800	0.09427200
H	1.54053700	-0.51025300	1.06214500
O	-1.11068600	-0.64427900	0.02943800

3(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.06486300	1.29850200	-0.11294500
C	0.20074800	-1.36788100	-0.04088800
C	-1.37224500	0.53246500	0.11245900
H	-0.00717800	1.73456900	-1.11373400
H	0.09069400	2.08389000	0.62866300
H	-2.14953500	0.82095200	-0.60212200
H	-1.75845800	0.68130500	1.12887000
N	-1.04214300	-0.91160700	-0.06501800
H	-1.80709300	-1.57779200	-0.07838600
S	1.27154600	-0.00876200	0.04625500

3(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.02390500	1.24644400	0.15154700
C	-0.01780500	-1.28475700	-0.18700200
C	1.31486200	0.56749100	-0.24241400
H	-0.01586900	1.59940000	1.18734800
H	-0.27666300	2.08091300	-0.50803200
H	2.17124500	1.04227400	0.24758800
H	1.45642100	0.61289200	-1.32607200
N	1.23965100	-0.85760500	0.15158500
H	1.51572700	-1.00935000	1.12756800
S	-1.32295800	-0.09362300	-0.00764200

4(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.04120100	1.29823900	0.18167000
C	0.10317500	-1.41812100	0.10871000
C	-1.35974300	0.57952200	-0.13961900
H	0.09279400	2.17876800	-0.45154700
H	-0.01144100	1.61694200	1.22833600
H	-1.66470200	0.74130400	-1.18150300
H	-2.18877600	0.88150700	0.50984000
N	-1.09526800	-0.88343200	0.05827500
H	-1.91381900	-1.48674900	0.12217900
P	1.28131400	-0.02701300	-0.17545300
H	1.91971500	-0.10038900	1.09200400

4(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.03576600	1.21894700	-0.25879500
C	-0.01529000	-1.27782600	-0.23379400
C	1.30883100	0.63048600	0.21073300
H	-0.27686700	2.14935000	0.26537200
H	-0.01733600	1.42419800	-1.33424500
H	1.42065600	0.77480200	1.29522800
H	2.15965000	1.10494700	-0.29177500
N	1.28347900	-0.82036300	-0.10661100
H	1.92962500	-1.39120000	0.43464700
P	-1.36095800	-0.11719600	0.03908700
H	-1.33236400	0.00873900	1.48188200

5(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.04058300	1.35625600	-0.00029800
C	-0.03172100	-1.49783000	-0.00019000
C	1.38610000	0.60915700	0.00016300
H	-0.05295800	1.99799800	0.88134800
H	-0.05236800	1.99808800	-0.88191600
H	1.99178100	0.83069000	0.88634700
H	1.99236400	0.83077500	-0.88560100
N	1.12491600	-0.88928100	0.00000500
H	1.98436800	-1.44461500	-0.00010100
Si	-1.27288600	-0.05024000	0.00005200
H	-2.14418100	-0.04537600	-1.20677000
H	-2.14278700	-0.04474300	1.20788700

5(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.00452700	1.27955100	-0.16873000
C	0.02737800	-1.35639300	0.03611200
C	1.34899600	0.60966600	0.21018300
H	-0.17066200	2.17554600	0.43550200
H	0.01862600	1.58451800	-1.22291600
H	1.50062500	0.67391600	1.29927100
H	2.20383300	1.08218200	-0.28656600
N	1.27604600	-0.81283800	-0.21544800
H	2.08890400	-1.37823300	0.01565500
Si	-1.31832800	-0.10450000	0.04195800
H	-2.29097900	-0.14198700	-1.08741600
H	-2.11149100	-0.04001000	1.30179900

6a(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.63673300	1.04538300	-0.11469800
C	1.20964900	-0.39025800	0.08350900
C	0.06103700	-1.37639700	-0.05656400
C	-0.87448200	0.85883100	0.09749400
H	0.83462500	1.39616800	-1.13359900
H	1.06232600	1.77867800	0.57667400
H	-1.49595500	1.37506500	-0.64182300
H	-1.20842200	1.15839500	1.09927800
N	-1.01386500	-0.61957600	-0.04962800
H	-1.94162200	-1.03030700	-0.09005300
H	2.02011600	-0.63162100	-0.61282500
H	1.62836500	-0.53470200	1.09130100

6a(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.64671100	0.97513900	-0.19312800
C	-1.26601200	-0.41843100	0.13523000
C	-0.05876200	-1.27927600	-0.03841000
C	0.84073600	0.82718100	0.18524600
H	-1.13352400	1.79331700	0.34738400
H	-0.73510000	1.16898500	-1.26758700
H	0.97604600	0.98208000	1.26768300
H	1.49212900	1.52281000	-0.35387900
N	1.14146300	-0.57362500	-0.20042300
H	1.96017300	-0.97249400	0.25260500
H	-2.09546900	-0.66738200	-0.53924800
H	-1.67001100	-0.43961600	1.16237800

6b(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.36097100	1.19151700	0.17479300
C	0.61997800	-0.01277400	-0.02725200
C	-0.23177000	-1.15777000	-0.58832200
C	-1.74920500	0.54132900	0.23623800
H	-0.30517000	1.86878400	-0.68584400
H	-0.13556500	1.77679200	1.07257600
H	-2.52181000	1.08328700	-0.31970500
H	-2.11078100	0.38283900	1.26038300
N	-1.47455300	-0.77548700	-0.40513700
H	-2.25068700	-1.38394900	-0.64873400
C	1.18806700	-0.50449900	1.32435400
H	1.84064400	0.26281600	1.76047600
H	0.39034900	-0.72158800	2.04589700
H	1.77282800	-1.42049700	1.18807400
C	1.77407400	0.33041500	-0.98104800
H	2.37308400	1.16007100	-0.58209100
H	2.42973500	-0.53597800	-1.11967200
H	1.39820200	0.62653000	-1.96798900

6b(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.32195000	0.16909900	1.14531500
C	0.66298000	-0.03630500	-0.05914200
C	-0.32131800	-0.60835900	-1.04264200
C	-1.71265800	0.36133400	0.50985000
H	-0.03145500	1.01724500	1.77547800
H	-0.32641900	-0.73455700	1.76572600
H	-1.85597400	1.40649100	0.19398700
H	-2.53136200	0.08558700	1.18275600
N	-1.66476700	-0.55346500	-0.65580100
H	-2.33878600	-0.35056800	-1.38994900
C	1.25149400	1.31584000	-0.53305900
H	0.46141900	2.04725200	-0.73817300
H	1.92190700	1.73812700	0.22885300
H	1.82748500	1.18109000	-1.45585900
C	1.81071000	-0.99983000	0.29417400
H	2.44862500	-1.17824000	-0.57967000
H	2.44142400	-0.58207000	1.09033500
H	1.42095400	-1.96678200	0.63013900

6c(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.42999000	1.19733200	-0.11149700
C	0.51426200	-0.02447500	-0.05360000
C	-0.27604500	-1.28384100	-0.09971800
C	-1.82242900	0.57330300	0.10840000
C	1.77547900	-0.04209700	0.81047400
C	1.89773500	-0.00378800	-0.68006200
H	-0.37676700	1.68231800	-1.09344800
H	-0.19845700	1.95354500	0.64568700
H	-2.56577800	0.88628800	-0.63277000
H	-2.22910000	0.77155900	1.10800700
H	2.01040200	-0.96827500	1.32667700
H	1.98984400	0.86548500	1.37044100
H	2.21968400	-0.90374900	-1.19619800
H	2.20488700	0.93037800	-1.14580800
N	-1.53052600	-0.88120800	-0.03038600
H	-2.29510900	-1.54769800	-0.01386800

6c(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.38178500	1.12373700	-0.28106500
C	-0.56351800	-0.07829200	-0.06859400
C	0.38204300	-1.20371700	-0.08348700
C	1.74438100	0.61560800	0.23556700
C	-1.96330000	-0.10985300	-0.63784900
C	-1.77496900	0.00188100	0.85816700
H	0.04810800	2.02459300	0.24437500
H	0.45171500	1.35022700	-1.35212700
H	1.80414800	0.73126300	1.32916300
H	2.59685700	1.12574300	-0.22395600
H	-2.32101500	-1.05374100	-1.04227100
H	-2.31041900	0.76927000	-1.17842100
H	-1.99629200	-0.86851900	1.47088500
H	-1.98940100	0.95758500	1.33399900
N	1.72755400	-0.81855500	-0.15363000
H	2.38488000	-1.40272000	0.35733000

6d(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.35393400	1.19640500	-0.00030100
C	-0.58244300	-0.05097200	-0.00016300
C	0.23976400	-1.30177400	-0.00015800
C	1.76896500	0.59393300	0.00032400
C	-1.95586500	-0.02626200	-0.64524200
C	-1.95572900	-0.02661800	0.64556000
H	0.18097300	1.82221900	0.88237700
H	0.18153300	1.82153800	-0.88357600
H	2.35625900	0.85546200	0.88825900

H	2.35710300	0.85581300	-0.88694300
H	-2.47170800	-0.01296300	-1.59419400
H	-2.47109100	-0.01219800	1.59474300
N	1.48466500	-0.87334900	-0.00010400
H	2.26252600	-1.52470100	-0.00005000

6d(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.34345800	1.13715500	-0.24631300
C	-0.63311800	-0.05648600	-0.04766400
C	0.29919800	-1.19605000	-0.03605200
C	1.70983900	0.59733600	0.22321500
C	-2.04665900	-0.08609300	-0.55739800
C	-1.92568100	0.01264100	0.73835600
H	0.02517300	2.02190000	0.31358300
H	0.38669100	1.39519200	-1.31189700
H	1.81458600	0.71168900	1.31326700
H	2.56182300	1.07816400	-0.26756100
H	-2.67832500	-0.28802500	-1.41441100
H	-2.38287300	-0.04827200	1.71865900
N	1.63925600	-0.83940400	-0.15644700
H	2.31590800	-1.44584000	0.29862300

6e(s)

	Coordinates (Angstroms)		
	X	Y	Z
N	2.14097700	-0.19839600	1.09667000
C	0.84383000	-0.04578100	1.22455900
C	0.32527200	0.17140100	-0.20229900
C	1.59629600	0.42957500	-1.08192200
C	2.75879500	-0.13590800	-0.25751900
C	-0.65729200	1.36432900	-0.26860300
C	-1.98194000	1.11511000	0.46835700
C	-2.67129100	-0.16634700	-0.02363100
C	-1.73228500	-1.37608400	0.09177600
C	-0.40878700	-1.12739800	-0.64962400
H	1.52552400	-0.03306300	-2.07189000
H	1.73297400	1.50787800	-1.22962400
H	-0.61419200	-1.03508400	-1.72739400
H	0.25934400	-1.99263500	-0.53276100
H	-2.97566100	-0.03940700	-1.07502100
H	-3.59132300	-0.34585700	0.54855900
H	-0.86439000	1.57540700	-1.33011300
H	-2.64533900	1.98000700	0.33100200
H	-1.78227500	1.02860900	1.54363300
H	-1.52495900	-1.57635200	1.15010200
H	2.72558000	-0.40103500	1.90247700
H	-2.21506400	-2.27350400	-0.31901600
H	-0.16592500	2.26004400	0.13646800
H	3.64825600	0.50314600	-0.24078400
H	3.06502800	-1.14276100	-0.56888500

6e(t)

	Coordinates (Angstroms)		
	X	Y	Z
N	2.31251800	-0.07178600	1.13998100
C	0.91342600	-0.09138700	1.12743500
C	0.28031500	-0.15230700	-0.23839800
C	1.58510700	-0.34777300	-1.08466900
C	2.72194900	0.26459000	-0.24426600
C	-0.45266300	1.16589700	-0.61693900
C	-1.72585700	1.37535100	0.21676700
C	-2.68650300	0.18412600	0.07790000
C	-1.98640600	-1.14227000	0.41299300
C	-0.70459700	-1.33162400	-0.41341900
H	1.76730200	-1.42057700	-1.21932000
H	1.50574700	0.11356000	-2.07533700
H	-0.96763600	-1.41435900	-1.48031000
H	-0.20455000	-2.26644100	-0.13078600
H	-3.06363500	0.14310300	-0.95596900
H	-3.56273300	0.32492100	0.72479200
H	-0.72262500	1.11892200	-1.68454200
H	-2.22484600	2.30537600	-0.08672100
H	-1.44306500	1.49784200	1.27283600
H	-1.72357800	-1.15780900	1.48115800
H	2.74837000	0.49017700	1.86700800
H	-2.66895100	-1.98589300	0.24443100
H	0.22752800	2.01881000	-0.49567600
H	2.77413500	1.35437700	-0.39431700
H	3.70228400	-0.16713400	-0.47154300

7a(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	1.26552300	-0.15299600	-0.00030000
C	-1.05082900	1.02943400	-0.00003100
C	0.11071600	-1.16007900	0.00032800
H	1.92351700	-0.26565300	0.87358900
H	1.92238400	-0.26547800	-0.87508300
H	0.08237300	-1.80437500	0.88740900
H	0.08223100	-1.80544200	-0.88595300
N	-1.11227800	-0.28356100	-0.00020000
H	-2.01231800	-0.76778100	-0.00026400
B	0.54537700	1.25704900	0.00017400
H	1.10841000	2.31025200	0.00084300

7a(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.88932600	0.86731000	-0.06101500
C	0.09918900	-1.32728900	0.01157300
C	0.65732700	0.94994100	0.07457100
H	-1.38918300	1.48917000	0.69208900
H	-1.21353100	1.25173300	-1.03999900

H	0.95345400	1.31514200	1.06769500
H	1.13629300	1.58413800	-0.67966300
N	1.12288200	-0.45177600	-0.08570100
H	2.09498000	-0.70659500	0.04058600
B	-1.26120100	-0.70195100	0.05149100
H	-2.33931800	-1.20117400	0.11097400

7b(s)

	Coordinates (Angstroms)		
	X	Y	Z
C	-0.13698900	1.24321700	-0.00018900
C	-0.03844500	-1.37132500	-0.00010800
C	-1.53439300	0.59684800	0.00020300
H	0.00546100	1.88444100	-0.87966900
H	0.00580700	1.88495300	0.87885600
H	-2.13272200	0.84186500	-0.88592700
H	-2.13207000	0.84168900	0.88682700
N	-1.25621400	-0.88370800	-0.00003800
H	-2.07516300	-1.49388600	0.00000200
B	0.83705000	-0.03017800	-0.00006200
N	2.23259300	-0.04184400	0.00007000
H	2.74083800	-0.91882100	0.00022600
H	2.82690500	0.77707600	0.00033400

7b(t)

	Coordinates (Angstroms)		
	X	Y	Z
C	0.09736200	1.18097800	-0.13678900
C	0.10003900	-1.24517000	-0.01890600
C	1.50640800	0.60850100	0.16962800
H	-0.14089300	2.02084700	0.52779400
H	0.06200300	1.56742500	-1.16664800
H	1.74584800	0.74225500	1.23557700
H	2.30919800	1.05936100	-0.42406700
N	1.40763700	-0.84308500	-0.14242400
H	2.15875800	-1.44800600	0.17380300
B	-0.88631500	-0.09414300	-0.00626300
N	-2.29700800	-0.09253700	0.05999100
H	-2.84802100	-0.93883900	0.10887300
H	-2.85257700	0.75116200	0.06941300