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Conformational effects of 1,5,9-substitution in symmetric bicyclo[3.3.1]nonane analogues

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List of Tables

Results of calculations: optimal energy values (hartrees, E_h) and bond lengths (angstroms, Å). For **BC** structures, the upper non-convex cycle corresponds to the **B**-shaped cycle, and the convex lower — to the **C**-shaped one.

Table S1: MP2/cc-pVTZ results for optimized least energy conformers of hydrocarbons **1**–**3**: energy values (E_h) and bond lengths (Å)

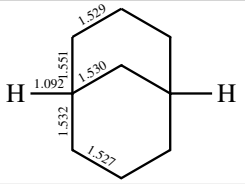
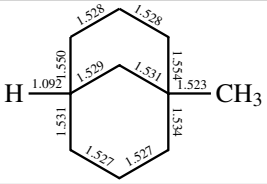
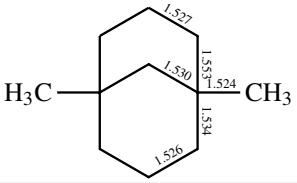
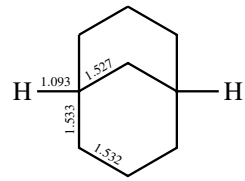
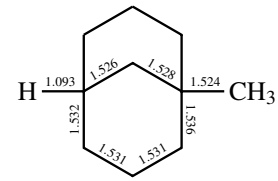
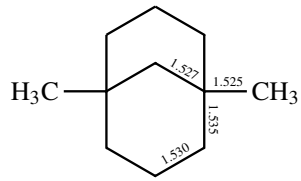
Str.	**1**	**2**	**3**
BC			
E_{MP2}	−351.798969	−391.027418	−430.255827
E_{ZPE}	0.237671	0.265225	0.292752
E_{tot}	−352.071633	−391.330191	−430.588739
E_{ϖ}	−351.833961	−391.064966	−430.295986
CC			
E_{MP2}	−351.802715	−391.031394	−430.260051
E_{ZPE}	0.237813	0.265288	0.292772
E_{tot}	−352.075137	−391.333878	−430.592594
E_{ϖ}	−351.837324	−391.068589	−430.299822

Table S2: MP2/cc-pVTZ results for optimized least energy conformers of ketones **4–6**: energy values (E_h) and bond lengths (Å)

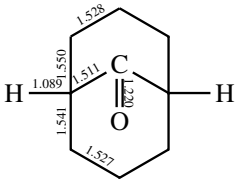
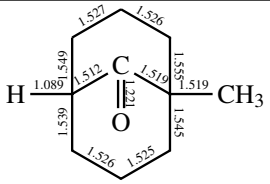
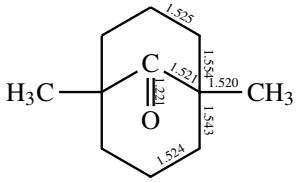
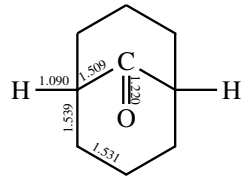
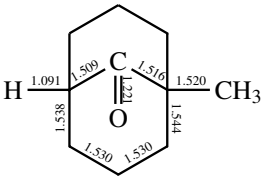
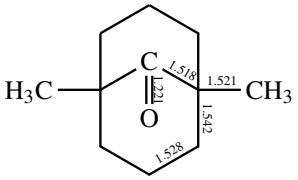
Str.	**4**	**5**	**6**
BC			
E_{MP2}	−425.722570	−464.951286	−504.179696
E_{ZPE}	0.218184	0.245960	0.273714
E_{tot}	−426.023055	−465.281474	−504.539752
E_{ϖ}	−425.804870	−465.035514	−504.266038
CC			
E_{MP2}	−425.723948	−464.952679	−504.181119
E_{ZPE}	0.218308	0.245985	0.273633
E_{tot}	−426.024504	−465.282968	−504.541269
E_{ϖ}	−425.806196	−465.036983	−504.267635

Table S3: MP2/cc-pVTZ results for optimized least energy conformers of aza derivatives **7–9**: energy values (E_h) and bond lengths (Å)

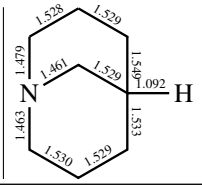
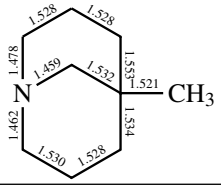
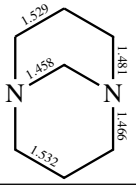
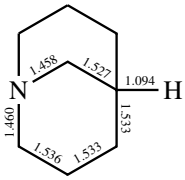
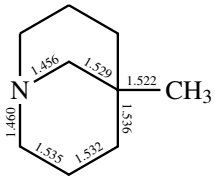
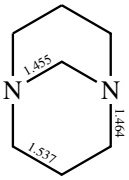
Str.	**7**	**8**	**9**
BC			
E_{MP2}	−367.812072	−407.040855	−383.829187
E_{ZPE}	0.225901	0.253431	0.214436
E_{tot}	−368.087998	−407.346929	−384.108452
E_{ϖ}	−367.862097	−407.093498	−383.894016
CC			
E_{MP2}	−367.817678	−407.046364	−383.835837
E_{ZPE}	0.225983	0.253490	0.214447
E_{tot}	−368.093111	−407.352166	−384.114835
E_{ϖ}	−367.867127	−407.098676	−383.900388

Table S4: Simplest BSR reagents from MP2 / cc-pVTZ optimization: energy values (E_h) and distances (Å).

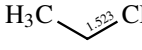
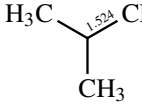
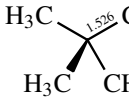
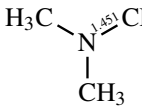
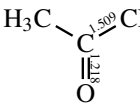
Structure	Energy, E_h	
 **10** ($\mathbb{C}_{2v}$)	E_{MP2}	−118.851739
	E_{ZPE}	0.104627
	E_{tot}	−118.957012
	E_{ϖ}	−118.852385
 **11** ($\mathbb{C}_{3v}$)	E_{MP2}	−158.076534
	E_{ZPE}	0.132857
	E_{tot}	−158.213107
	E_{ϖ}	−158.080249
 **12** ($\mathbb{T}_d$)	E_{MP2}	−197.303360
	E_{ZPE}	0.160632
	E_{tot}	−197.470495
	E_{ϖ}	−197.309863
 **13** ($\mathbb{C}_{3v}$)	E_{MP2}	−174.086656
	E_{ZPE}	0.121647
	E_{tot}	−174.226450
	E_{ϖ}	−174.104803
 **14** ($\mathbb{C}_{2v}$)	E_{MP2}	−192.774722
	E_{ZPE}	0.084169
	E_{tot}	−192.909172
	E_{ϖ}	−192.825003

Table S5: Bond reference (prototype) compounds for the BSRs from MP2 / cc-pVTZ optimization: energy values (E_h) and distances (Å).

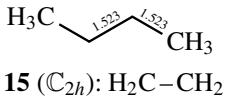
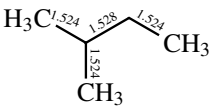
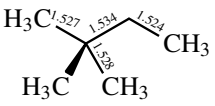
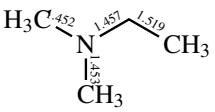
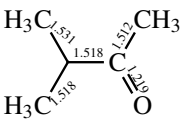
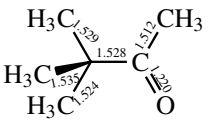
Structure	Energy, E_h	
 **15** ($\mathbb{C}_{2h}$): H_2C-CH_2	E_{MP2}	−158.073762
	E_{ZPE}	0.133345
	E_{tot}	−158.210782
	E_{ϖ}	−158.077437
 **16**: $HC-CH_2$	E_{MP2}	−197.297895
	E_{ZPE}	0.161615
	E_{tot}	−197.465969
	E_{ϖ}	−197.304355
 **17** ($\mathbb{C}_s$): $C-CH_2$	E_{MP2}	−236.523765
	E_{ZPE}	0.189566
	E_{tot}	−236.722328
	E_{ϖ}	−236.532762
 **18**: $N-CH_2$	E_{MP2}	−213.310039
	E_{ZPE}	0.150339
	E_{tot}	−213.481323
	E_{ϖ}	−213.330983
 **19**: $HC-CO$	E_{MP2}	−271.220682
	E_{ZPE}	0.142084
	E_{tot}	−271.417479
	E_{ϖ}	−271.275395
 **20**: $C-CO$	E_{MP2}	−310.445989
	E_{ZPE}	0.170203
	E_{tot}	−310.673169
	E_{ϖ}	−310.502967

Table S6: Molecular strain estimates for the least-energy conformers, $\text{kcal} \cdot \text{mol}^{-1}$

Structure and its hyperhomodesmotic bond separation reaction			$\mathscr{E}_{\varsigma}$, $\text{kcal} \cdot \text{mol}^{-1}$	
			BC	**CC**
(**1**)	+ 7 (**10**) + 4 (**11**)	→ 4 (**15**) + 6 (**16**)	8.923	6.813
(**2**)	+ 7 (**10**) + 2 (**11**) + 2 (**12**)	→ 4 (**15**) + 3 (**16**) + 3 (**17**)	5.780	3.506
(**3**)	+ 7 (**10**) + 4 (**12**)	→ 4 (**15**) + 6 (**17**)	2.627	0.220
(**4**)	+ 6 (**10**) + 4 (**11**) + (**14**)	→ 4 (**15**) + 4 (**16**) + 2 (**19**)	8.015	7.183
(**5**)	+ 6 (**10**) + 2 (**11**) + 2 (**12**) + (**14**)	→ 4 (**15**) + 2 (**16**) + 2 (**17**) + (**19**) + (**20**)	4.574	3.652
(**6**)	+ 6 (**10**) + 4 (**12**) + (**14**)	→ 4 (**15**) + 4 (**17**) + 2 (**20**)	1.208	0.206
(**7**)	+ 7 (**10**) + 2 (**11**) + 2 (**13**)	→ 4 (**15**) + 3 (**16**) + 3 (**18**)	10.581	7.425
(**8**)	+ 7 (**10**) + 2 (**12**) + 2 (**13**)	→ 4 (**15**) + 3 (**17**) + 3 (**18**)	7.189	3.940
(**9**)	+ 7 (**10**) + 4 (**13**)	→ 4 (**15**) + 6 (**18**)	9.865	5.866