Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Steric effects of the alkyl groups: evaluation the isolated molecules by means of isodesmic reactions

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Supplementary information

Table S1 DFT-Energies of alkyl substituted cyclopropanes **1**, **3** and cyclopentanes **4**, **5** (in a. u.)

Substituents	**1** *cis*-1,2-cyclopropane	**3** *trans*-1,2-cyclopropane	**4** *cis*-1,2-cyclopentane	**5** *trans*-1,2-cyclopentane
H H	–117.9309084		–196.6116632	
H Me	–157.2579373		–235.9377095	
H Et	–196.5823742		–275.2587061	
H Pr	–235.906735			
H *i*-Bu	–275.2306824			
H *neo*-Pe	–314.5535534		–393.2299465	
H *i*-Pr	–235.9075789		–314.5826418	
H *t*-Bu	–275.2290857		–353.9057662	
Me Me	–196.5826017	–196.5848101	–275.2600556	–275.2633460
Me Et	–235.9068233	–235.9092505	–314.5834383	–314.5866148
Me Pr	–275.2312052	–275.2335868		

Me *i*-Bu	–314.5549981	–314.5575471		
Me *neo*-Pe	–353.8778981	–353.8804087	–432.5519854	–432.5476252
Me *i*-Pr	–275.2317861	–275.2343981	–353.9019984	–353.9081660
Me *t*-Bu	–314.5049389	–314.555796	–393.2239381	–393.2296127
Et Et	–275.2311635	–275.2336602	–353.9060772	–353.9097884
Et Pr	–314.5555084	–314.5580064		
Et *i*-Bu	–353.8792602	–353.8820322		
Et *neo*-Pe	–393.2021895	–393.2048485	–471.8746934	–471.8704767
Et *i*-Pr	–314.5560613	–314.5556904	–393.2251787	–393.2312672
Et *t*-Bu	–353.8735852	–353.8802601	–432.5460661	–432.5530201
Pr Pr	–353.879844	–353.8823401		
Pr *i*-Bu	–393.2036229	–393.2063146		
Pr *neo*-Pe	–432.5259809	–432.5292031		
Pr *i*-Pr	–353.8804486	–353.8831679		
Pr *t*-Bu	–393.1979447	–393.2045995		
i-Bu *i*-Bu	–432.5273466	–432.5302497		
i-Bu *neo*-Pe	–471.8502939	–471.8531451		
i-Bu *i*-Pr	–393.2042189	–393.2071578		
i-Bu *t*-Bu	–432.5214537	–432.5286076		
neo-Pe *neo*-Pe	–511.1731775	–511.1759038	–589.8429021	–589.8316209
neo-Pe *i*-Pr	–432.5242375	–432.5288875	–511.1940703	–511.1926087
neo-Pe *t*-Bu	–471.8445368	–471.8514264	–550.5091423	–550.5122386
i-Pr *i*-Pr	–353.8796818	–353.8839116	–432.5440522	–432.5529357
i-Pr *t*-Bu	–393.1974788	–393.2052741	–393.2239381	–471.8742854
t-Bu *t*-Bu	–432.5109815	–432.5266948	–511.1755161	–511.1916306

Table S2 Calculated energies of bicyclo[2.2.2]octane derivatives **2** and **6**

Substituent	1-alkyl-BCO	**2**	**6**
		1-alkyl-trimethyl-BCO	1-alkyl-hexamethyl-BCO
H	–313.3717029[a]	–431.3438193	–549.2609652
Me	–352.6984378[a]	–470.6634205	–588.5818250
Et	–392.0191784	–509.9777481	–627.8932125
Pr	–431.3433483	–549.3019033	–667.2172984
i-Bu	–470.6639327	–588.6191907	–706.5331578
neo-Pe	–509.9818325	–627.9315463	–745.8389234
i-Pr	–431.3393120	–549.2914039	–667.1987679
t-Bu	–470.6583232[a]	–588.6035611	–706.5002708

Table S3 Some calculated geometrical parameters of bicyclo[2.2.2]octane derivatives **2** and **6**

Compoundt	C1–C2			∠ C(X)-C1-C2			∠C1-C2-C(H_3)					
2 H	1.552	1.552	1.552				114.1	114.1	114.1			
2 Me	1.565	1.565	1.565	111.0	111.0	111.0	115.6	115.6	115.6			
2 Et	1.570	1.572	1.575	108.9	112.1	113.3	115.7	116.3	118.1			
2 Pr	1.569	1.573	1.576	108.9	112.1	113.3	115.9	116.3	118.1			
2 *i*-Bu	1.566	1.572	1.575	107.9	112.1	113.0	114.9	115.6	116.8			
eo-Pe	1.570	1.571	1.588	104.4	113.3	116.3	115.5	115.9	116.9			
2 *i*-Pr	1.570	1.573	1.578	109.9	111 3	112.9	115.0	115.8	117.4			
2 *t*-Bu	1.583	1.583	1.583	112.1	112.1	112.1	116.8	116.8	116.8			
6 H	1.594	1.594	1.594				111.9	115.2	111.9	115.2	111.9	115.2
6 Me	1.620	1.620	1.620	110.6	110.6	110.6	113.8	116.3	113.8	116.3	113.8	116.3
6 Et	1.620	1.624	1.638	106.8	112.7	113.9	114.3	116.9	114.5	116.3	115.3	115.9
6 Pr	1.622	1.622	1.637	107.0	112.2	114.1	113.8	117.2	114.8	115.7	115.0	115.9
6 *i*-Bu	1.624	1.625	1.645	105.8	113.8	114.4	114.3	117.3	115.0	116.0	115.5	116.1
6 *neo*-Pe	1.620	1.632	1.651	104.0	113.4	117.3	114.3	115.7	115.4	115.6	115.5	116.6
6 *i*-Pr	1.624	1.641	1.650	109,2	111.3	115.1	114.3	117.3	114.6	116.9	114.9	116.7
6 *t*-Bu	1.657	1.657	1.657	112.8	112.8	112.8	116.6	117.3	116.6	117.3	116.6	117.3