Supplementary Material for Organic & Biomolecular Chemistry

Steric effects of the polar substituents evaluated in terms of energy by means of isodesmic reactions

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Supplementary information

Table S1 DFT-calculated energies of sterically crowded cyclopropane derivatives **1** to **3** (in a. u.)

Substituent	**1** ΔE	**2** ΔE	**3** ΔE
H	–117.9309084	–275.2290857	–157.2579373
C≡CH	–194.0948265	–351.3899348	–233.4216306
CF_3	–455.0862038	–612.3762048	–494.4105586
CN	–210.1977365	–367.4941312	–249.5251671
$Si(CH_3)_3$	–526.6697711	–683.9591712	–565.9935877
NH_2	–173.2968432	–330.5892632	–212.6225809
NO_2	–322.4977465	–479.7883340	–361.8227074
OH	–193.1677423	–350.4662822	–232.4971684
OCH_3	–232.4818905	–389.7770680	–271.8074088
SO_2CH_3	–705.9051243	–863.1953047	–745.2297445
F	–217.1957774	–374.4917291	–256.5221648
Cl	–577.5531000	–734.8471926	–616.8794002
$C≡C^-$	–193.4788957	–350.7782931	–232.8062814
CO_2^-	–306.0096953	–463.3044223	–345.3349930
NH_3^+	–173.6553086	–330.9564492	–212.9840522
$N(CH_3)_3^+$	–291.6233002	–448.9093220	–231.8953720
O^-	–192.5670923	–349.8696834	–231.8953723

Table S2 DFT-calculated bond angles in sterically crowded cyclopropane derivatives **2** and **3**

Substituent	**2** ϑ_1 = ∠X-C1-C2	**2** ϑ_2 = ∠C1-C2-C	**3** ϑ_1 = ∠X-C1-C2	**3** ϑ_2 = ∠C1-C2-C
H		124.5		120.4
C≡CH	124.8	126.9	121.3	121.4
CF_3	128.0	131.2	123.5	124.2
CN	123.6	126.5	120.3	121.3
$Si(CH_3)_3$	136.1	129.7	128.7	123.3
NH_2	124.1	128.9	124.6	122.1
NO_2	123.0	129.4	119.9	123.7
OH	118.8	126.4	120.2	121.4
OCH_3	119.2	126.3	120.2	121.6
SO_2CH_3	127.9	131.1	124.7	124.7
F	119.6	126.1	117.8	121.0
Cl	124.3	128.9	121.2	122.9
$C\equiv C^-$	124.1	126.3	121.9	120.4
CO_2^-	124.9	131.1	121.9	122.3
NH_3^+	121.5	126.1	119.1	123.0
$N(CH_3)_3^+$	133.1	128.9	128.5	128.7
O^-	123.4	124.5	122.4	117.9