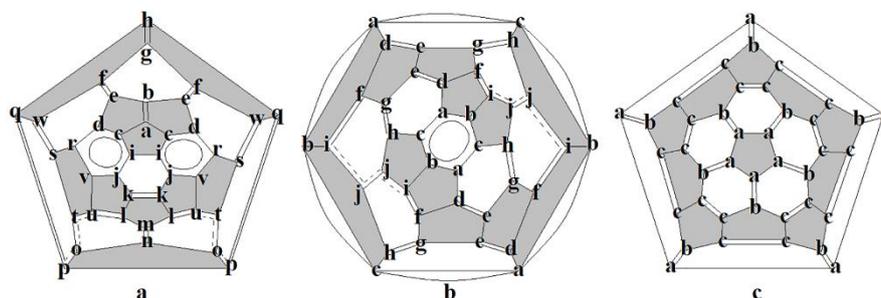


**The key feature of instability of small non-IPR closed-shell fullerenes:
three isomers of C₄₀**

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**Figure S1** Atom designation in molecules of isomers 31 (C_s) (a), 38 (D_2) (b) and 39 (D_{5d}) (c) of fullerene C_{40} for Table S1, S2.**Table S1** Calculated bonds lengths in singlet configurations of isomers 31 (C_s), 38 (D_2) and 39 (D_{5d}) of fullerene C_{40} .

| single bonds* | value | double bonds | value | delocalized bonds | value |
|------------------------|--------|--------------|--------|-------------------|--------|
| isomer 31 (C_s) | | | | | |
| a-c | 1.4568 | a-b | 1.3747 | c-d | 1.4299 |
| b-e | 1.4787 | e-f | 1.3729 | c-i | 1.4253 |
| d-e | 1.4888 | g-h | 1.3752 | d-r | 1.4139 |
| f-g | 1.4779 | k-k | 1.3703 | i-j | 1.4168 |
| f-w | 1.4992 | l-u | 1.3790 | j-v | 1.4277 |
| h-q | 1.4643 | m-n | 1.4016 | r-v | 1.4149 |
| i-i | 1.5094 | p-q | 1.3953 | o-p | 1.4257 |
| j-k | 1.4648 | s-w | 1.3935 | o-t | 1.4222 |
| k-l | 1.4910 | | | t-u | 1.4363 |
| l-m | 1.4516 | | | | |
| n-o | 1.4802 | | | | |
| p-p | 1.4966 | | | | |
| q-w | 1.4434 | | | | |
| r-s | 1.4914 | | | | |
| s-t | 1.4692 | | | | |
| u-v | 1.4829 | | | | |
| isomer 38 (D_2) | | | | | |
| a-d | 1.4566 | d-e | 1.3696 | a-b | 1.4291 |
| b-i | 1.4871 | f-i | 1.3774 | a-c | 1.4261 |
| c-h | 1.4996 | g-h | 1.3972 | b-c | 1.4091 |
| d-f | 1.4921 | | | i-j | 1.4348 |
| e-e | 1.4914 | | | j-j | 1.4199 |
| e-g | 1.4655 | | | | |
| f-g | 1.4503 | | | | |
| h-j | 1.4738 | | | | |
| isomer 39 (D_{5d}) | | | | | |
| a-a | 1.4732 | a-b | 1.4090 | - | - |
| b-c | 1.4545 | c-c | 1.3707 | | |
| c-c | 1.4895 | | | | |

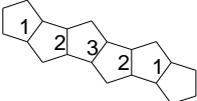
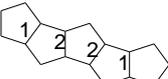
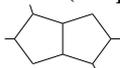
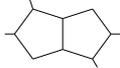
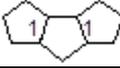
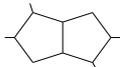
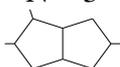
*bonds designation is according to Figure S1.

Table S2 Maximal dihedral angles (degree) in isomers 31 (C_s), 38 (D_2) and 39 (D_{5d}) of fullerene C_{40} .

| isomer no. | in hexagons with | | in pentagons |
|-----------------|------------------|--------------------------|--------------|
| | bond alternation | delocalized π -bonds | |
| 31 (C_s) | 21.90 (1) | 17.91 (2) | 10.24 (1) |
| 38 (D_2) | 9.72 (4) | 12.37 (2) | 8.79 (4) |
| 39 (D_{5d}) | 5.14 (10) | - | 13.67 (10) |

*numbers in parentheses represent the number of equivalent cycles according to the isomer symmetry.

Table S3 Dihedral angles and folding angles F (degree) of pentagonal fragments in molecules of isomers 31 (C_s), 38 (D_2) and 39 (D_{5d}) of fullerene C_{40} , isomers 4348 (C_{2v}) and 4169 (C_s) of fullerene C_{66} ²² and isomers 6140 (D_3) and 6275 (D_3) of fullerene C_{68} ²³.*

| Numbering of pentagon adjacencies in equivalent pentagonal fragments and their number (N) in molecule | Dihedral angles | | | F | |
|---|-----------------|---------|---------|-------|------|
| | a-b-b-a | c-b-b-c | average | | |
| C_{40} #38 (D_2) | | | | | |
| N = 2 | | | | | |
|  | 1 | 131.1 | 139.8 | 135.5 | 44.5 |
| | 2 | 137.2 | 128.3 | 132.8 | 46.2 |
| | 3 | 140.3 | 128.5 | 134.4 | 45.6 |
| C_{40} #31 (C_s) | | | | | |
| N = 1 | | | | | |
|  | 1 | 126.8 | 126.8 | 126.8 | 53.2 |
| | 2 | 124.2 | 128.8 | 126.5 | 53.5 |
| | 3 | 133.6 | 133.6 | 133.6 | 46.4 |
| N = 1 | | | | | |
|  | 1 | 137.4 | 133.8 | 135.6 | 44.4 |
| | 2 | 135.8 | 129.6 | 132.7 | 47.3 |
| N = 1 | | | | | |
|  | 1 | 125.6 | 125.6 | 125.6 | 54.4 |
| | 2 | 130.9 | 125.8 | 128.4 | 51.6 |
| C_{40} #39 (D_{5d}) | | | | | |
| N = 5 (loop) | | | | | |
|  | 1 | 124.7 | 141.9 | 133.3 | 46.7 |
| C_{66} #4348 (C_{2v}) | | | | | |
| N = 2 | | | | | |
|  | 1 | 133.7 | 133.7 | 133.7 | 46.3 |
| C_{66} #4169 (C_s) | | | | | |
| N = 1 | | | | | |
|  | 1 | 131.3 | 133.4 | 132.4 | 47.6 |
| C_{68} #6140 (D_3) | | | | | |
| N = 3 | | | | | |
|  | 1 | 130.6 | 136.3 | 133.5 | 46.5 |
| C_{68} #6275 (D_3) | | | | | |
| N = 3 | | | | | |
|  | 1 | 122.8 | 145.4 | 134.1 | 45.9 |

*References see in the main text.