

Supporting Information for
A structure–property interplay between width and height of cages
and static third order nonlinear optical responses for fullerenes:
applying gamma density analysis

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Table S1 The width and height (Å) of fullerenes.

Complex	Width h	Height
C ₄₀	5.54	4.83
C ₅₀	6.28	5.71
C ₆₀	6.59	6.60
C ₇₀	6.71	7.96
C ₂₄	4.45	3.18
C ₃₆	4.68	4.90
C ₄₈	6.22	4.75
C ₇₂	8.22	5.71

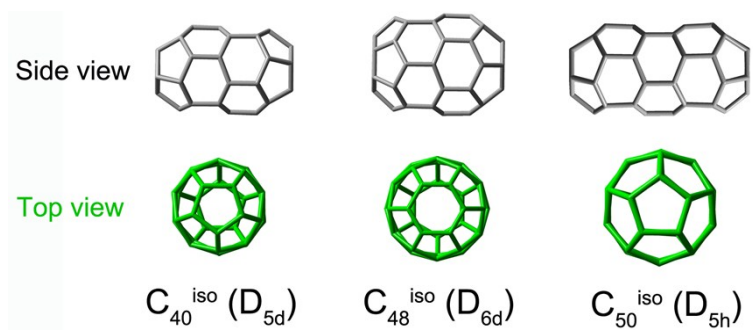


Fig. S1 The isomers of fullerenes C_{40} , C_{48} and C_{50} in their highest possible symmetries, which are D_{5d} , D_{6d} , and D_{5h} , respectively.