Supporting Information for the article

“Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colle-Salvetti Correlation Density Functionals”, submitted to the Journal of Chemical Theory and Computation

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Figure S1. Methane to ethane PES curve calculated by selected density functionals, relative to CCSD(T)/CBS computed values, kcal/mol. Intermolecule C-C distance in Angstroms.

Figure S2. Enhancement factors $F(x)$ for G96, B86, B88, OPTX, PBE and RGE2 density functionals.

Table S1. Deformation energies of isobutene to isobutene with CCC angles of 108°, computed by different methods, kcal/mol. Priroda DFT computations in the L11 basis set, MP2 in the L2 set.

Method	E_{def} , kcal/mol
BLYP	1.20
BPBE	1.13
OLYP	1.43
PBE	1.03
VWN5	0.77
B3LYP	1.19
PBE1	1.02
MP2/L2	0.86

Table S2. Energy differences between the eclipsed cis-transition state and the trans-conformer of n-butene, as the computed by different methods, kcal/mol. Priroda DFT computations in the L11 basis set, MP2 in the L2 set.

Method	E_{rot} , kcal/mol
BLYP	5.65
BPBE	5.69
OLYP	6.11
PBE	5.56
VWN5	5.53
B3LYP	5.79
PBE1	5.70
MP2/L2	5.75