Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Neural Network Atomistic Potentials for Global Energy Minima Search in Carbon Clusters

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Supplementary Figures

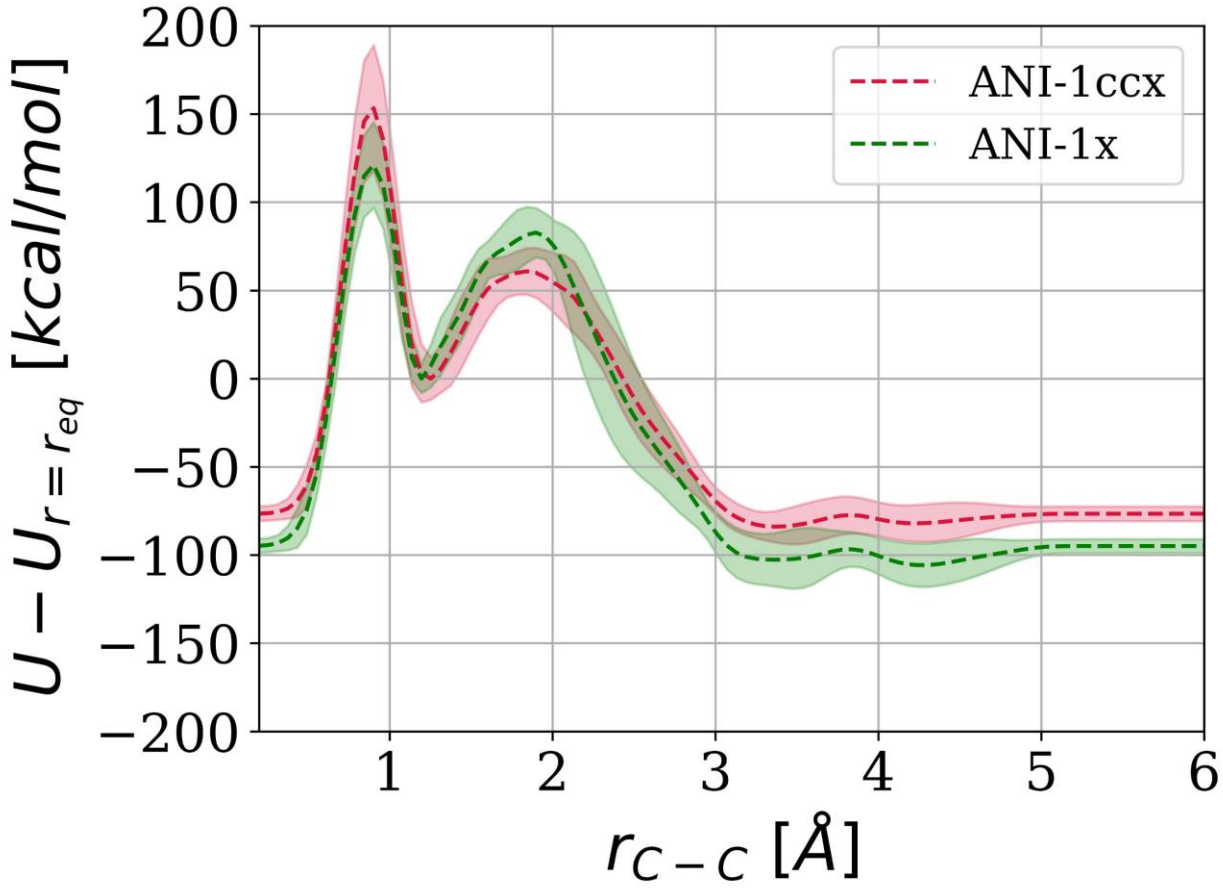

Figure S1. Potential energy surface of carbon dimer calculated using ANI-1ccx and ANI-1x models. Shaded regions show the ensemble standard deviation.

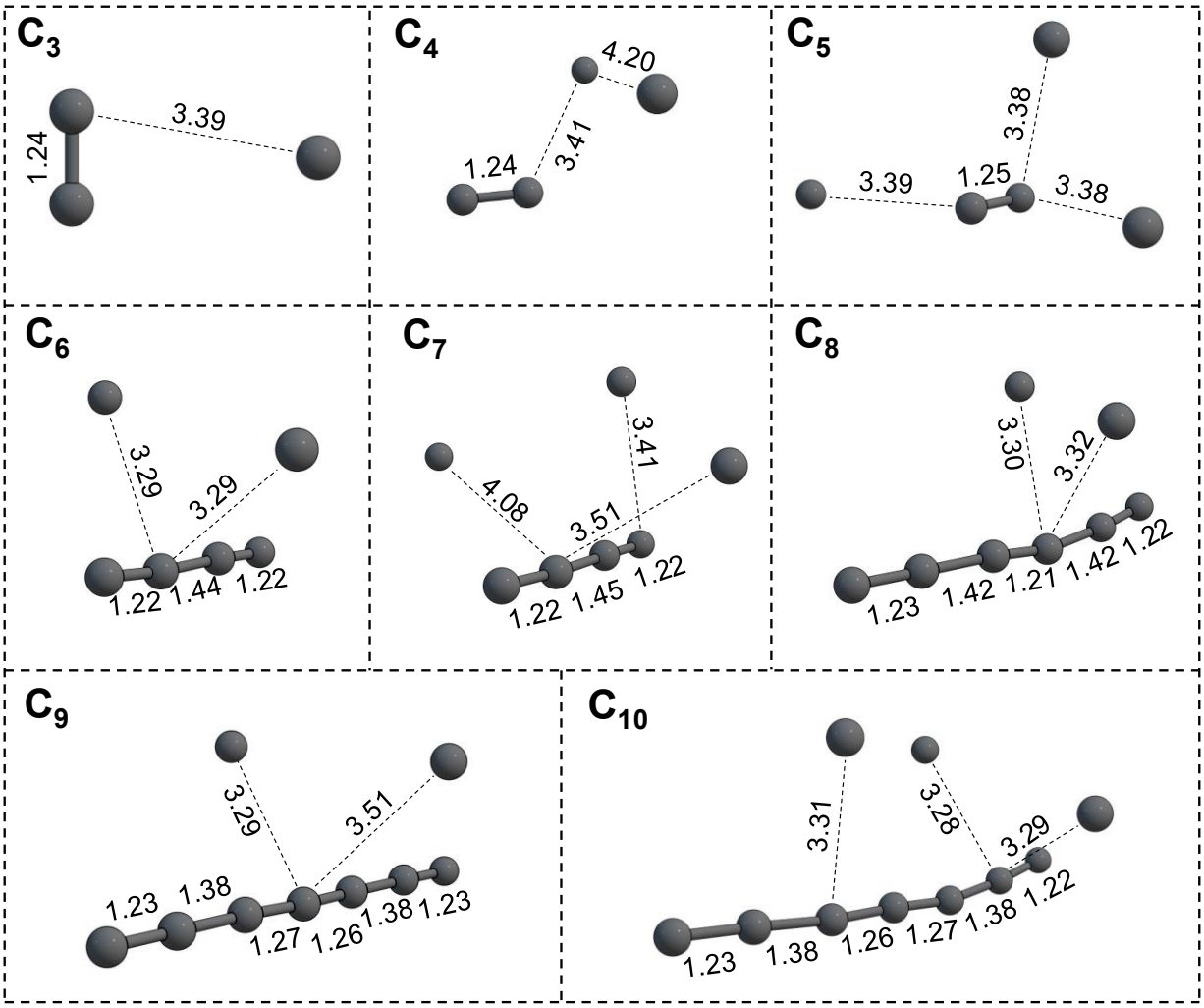

Figure S2. Global minimum structures of C_n (n = 3-10) clusters according to the ANI-1ccx method with the introduced proximity restriction.

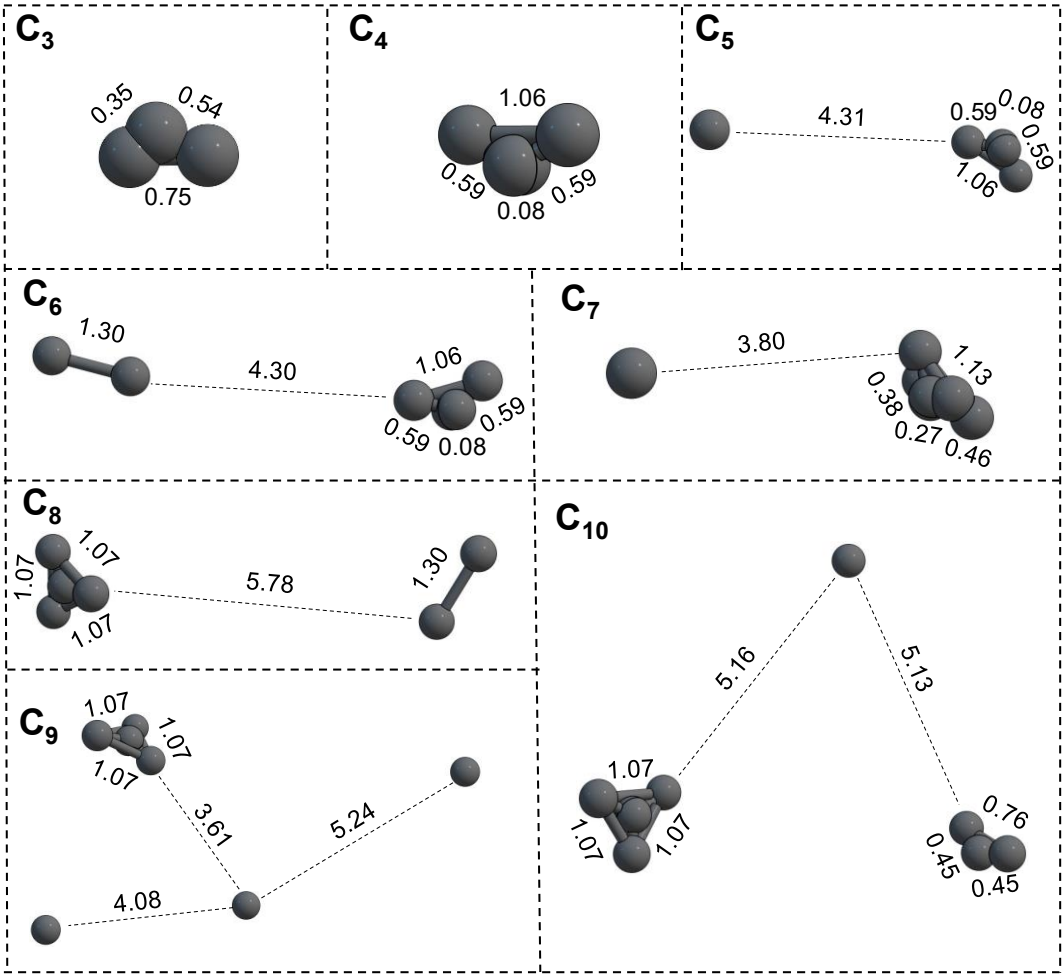

Figure S3. Global minimum structures of C_n (n = 3-10) clusters according to the ANI-nr method.

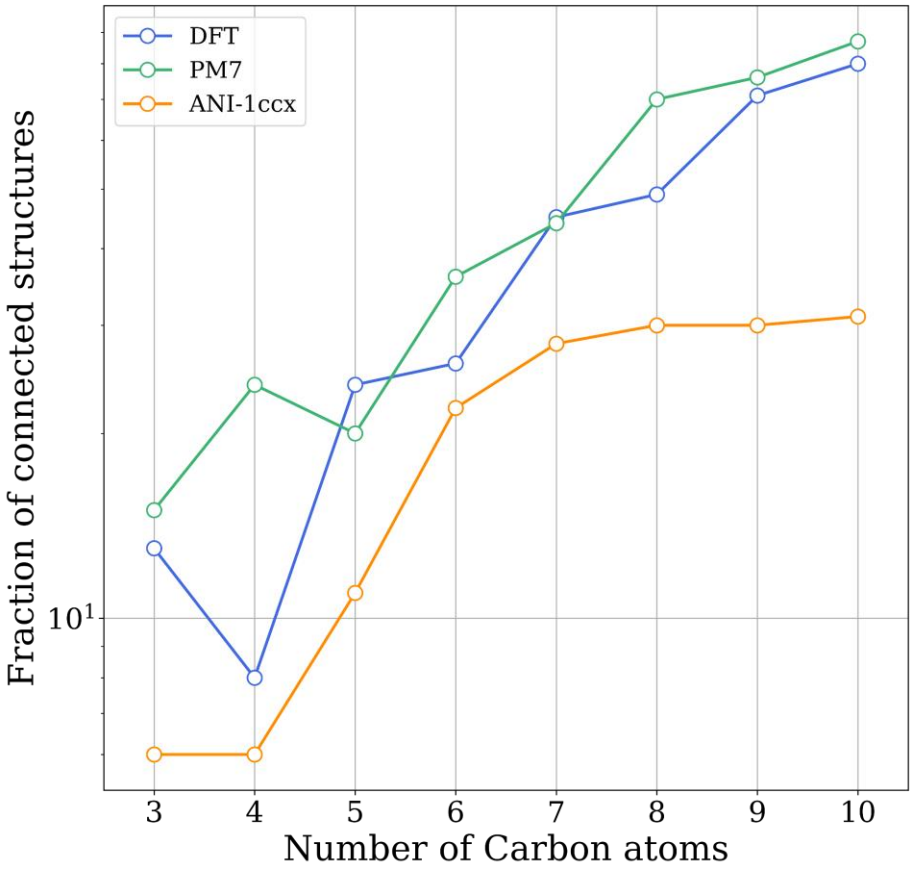

Figure S4. Number of connected structures with distinct energies for each method in case of undersampled PES (100 structures for each stoichiometry). Y-axis is in log-scale.

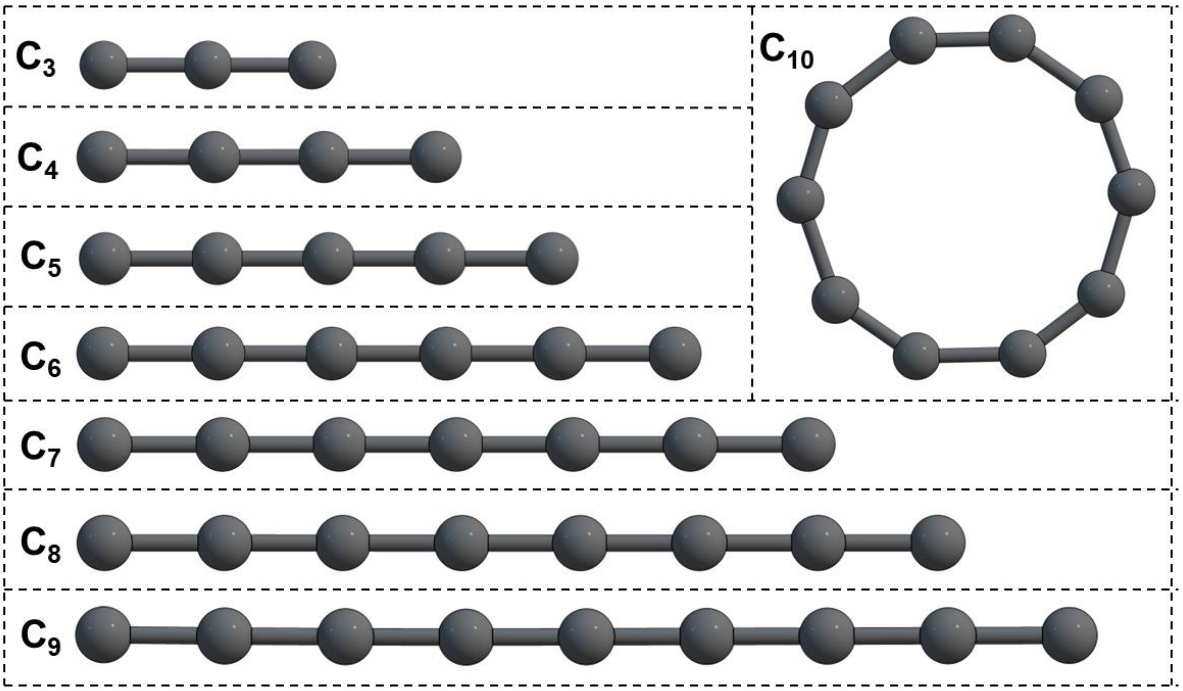

Figure S5. Global minimum structures of C_n (n = 3-10) clusters according to the PM7 method.

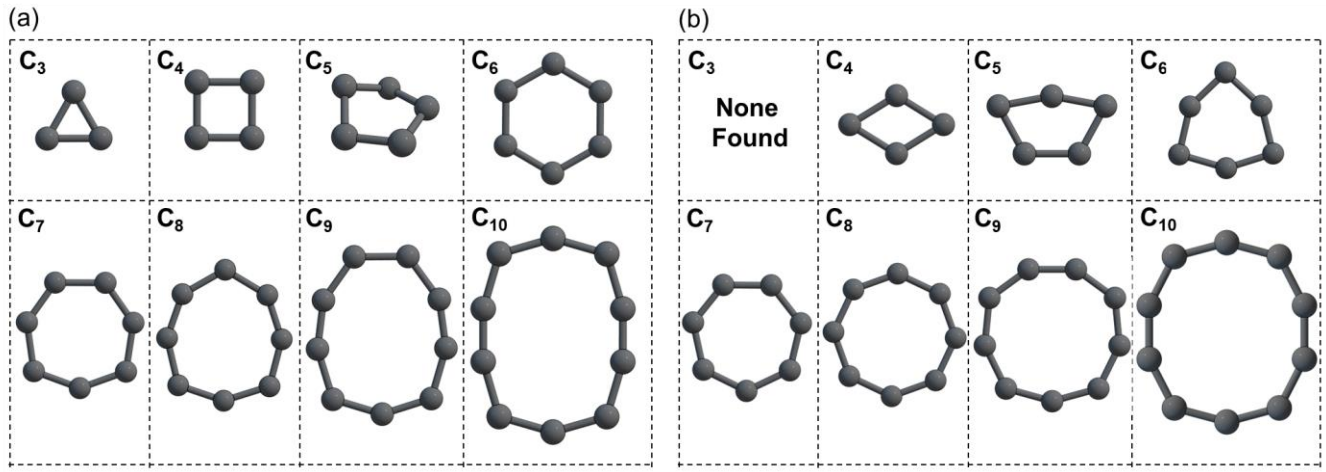

Figure S6. Lowest in energy cyclic structures of C_n (n = 3-10) clusters according to the ANI-1ccx (a) and ANI-nr (b) methods.

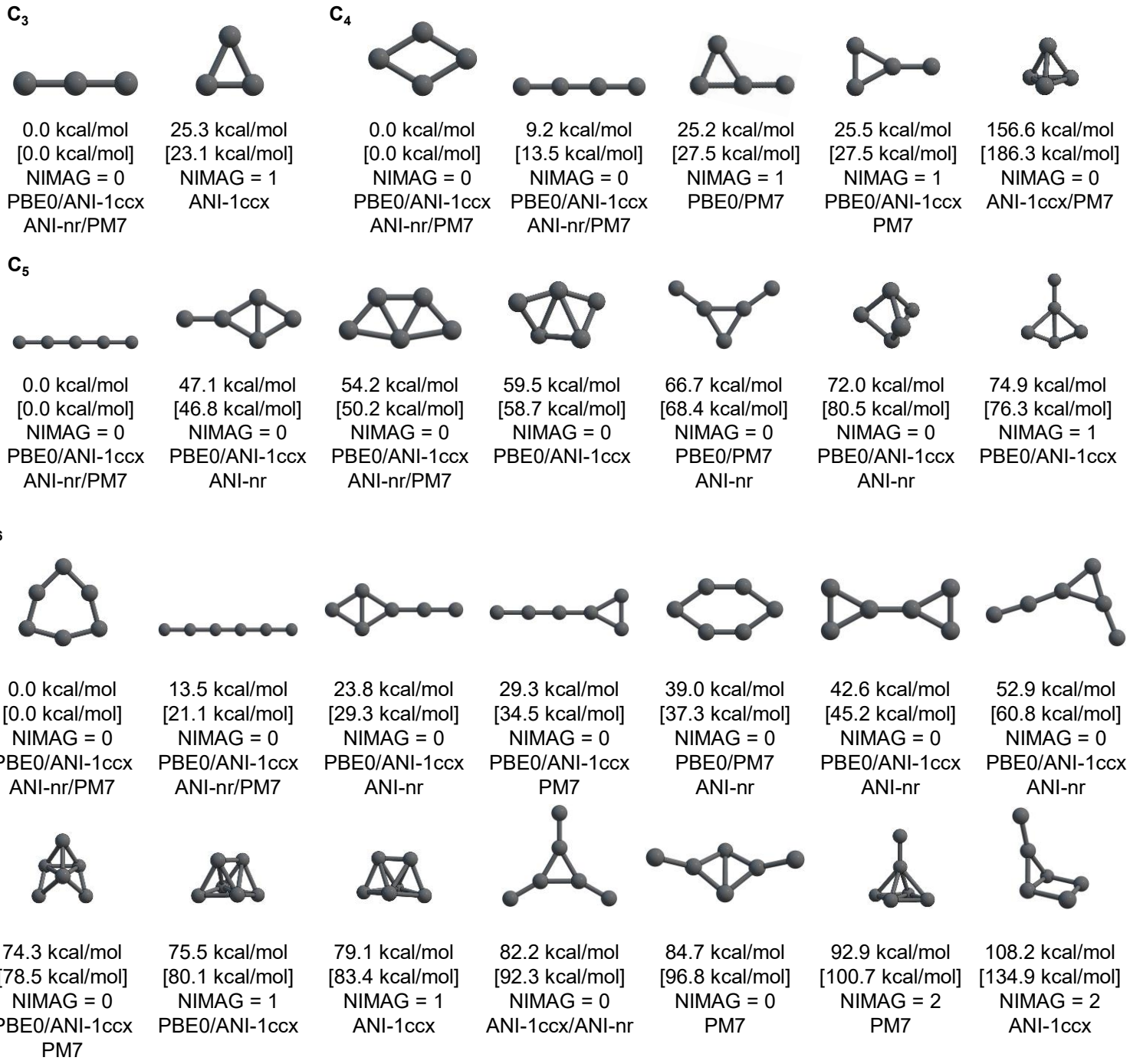

Figure S7. Optimized at PBE0/Def2-TZVPP level of theory geometries of lowest isomers of C_n (n = 3-6). The geometries obtained via reoptimization of ten initial guessed structures obtained by PBE0/def2-SVP, PM7, ANI-nr, and ANI-1ccx methods. The relative energies are given at CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level of theory. Relative energies in square brackets are calculated at PBE0/def2-TZVPP level. Number if imaginary frequencies (NIMAG) is given. Under each structure the method that provided the initial guess geometry is given.

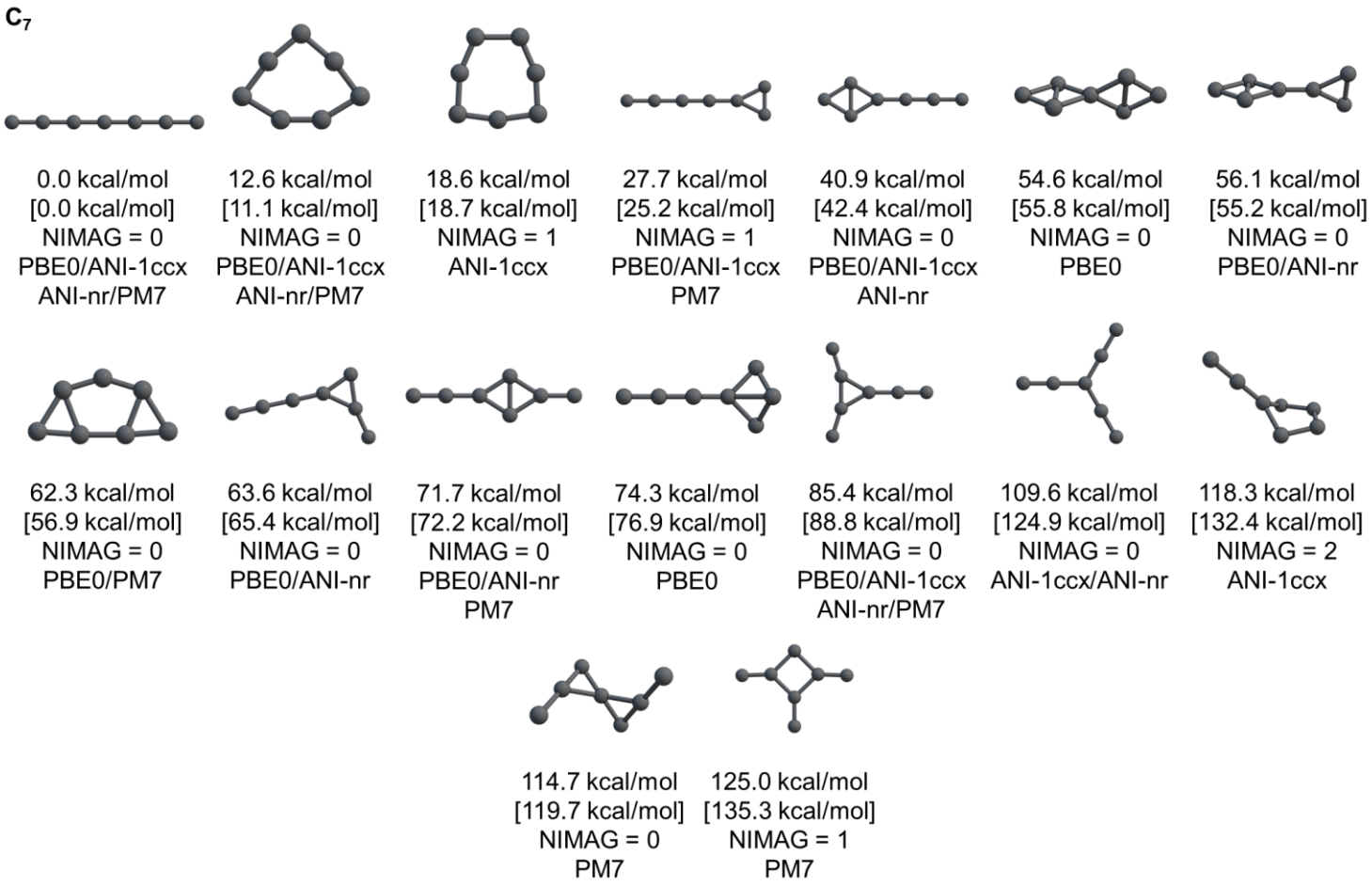

Figure S8. Optimized at PBE0/Def2-TZVPP level of theory geometries of lowest isomers of C_7. The geometries obtained via reoptimization of ten initial guessed structures obtained by PBE0/def2-SVP, PM7, ANI-nr, and ANI-1ccx methods. The relative energies are given at CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level of theory. Relative energies in square brackets are calculated at PBE0/def2-TZVPP level. Number if imaginary frequencies (NIMAG) is given. Under each structure the method that provided the initial guess geometry is given.

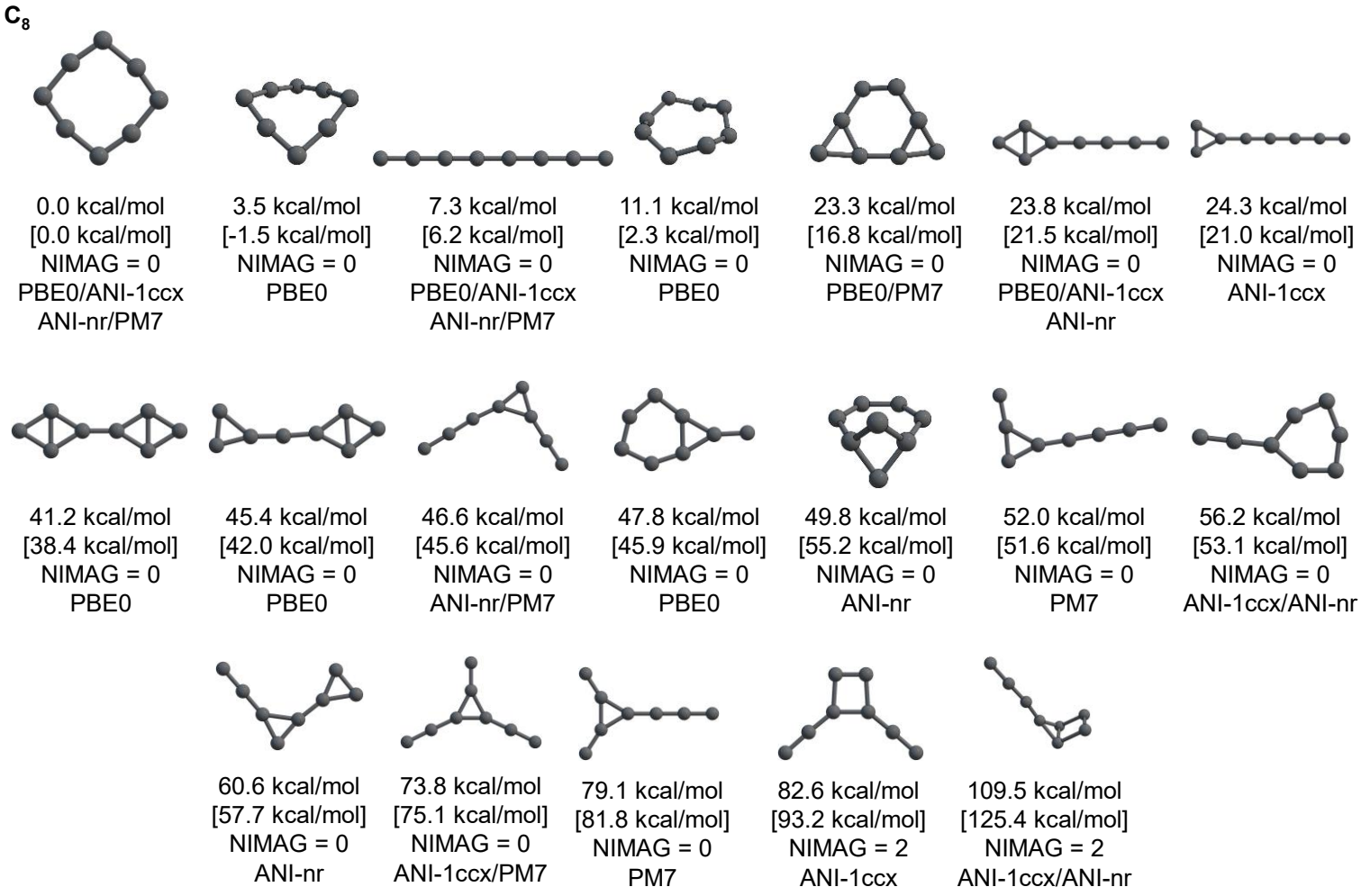

Figure S9. Optimized at PBE0/Def2-TZVPP level of theory geometries of lowest isomers of C_8. The geometries obtained via reoptimization of ten initial guessed structures obtained by PBE0/def2-SVP, PM7, ANI-nr, and ANI-1ccx methods. The relative energies are given at CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level of theory. Relative energies in square brackets are calculated at PBE0/def2-TZVPP level. Number if imaginary frequencies (NIMAG) is given. Under each structure the method that provided the initial guess geometry is given.

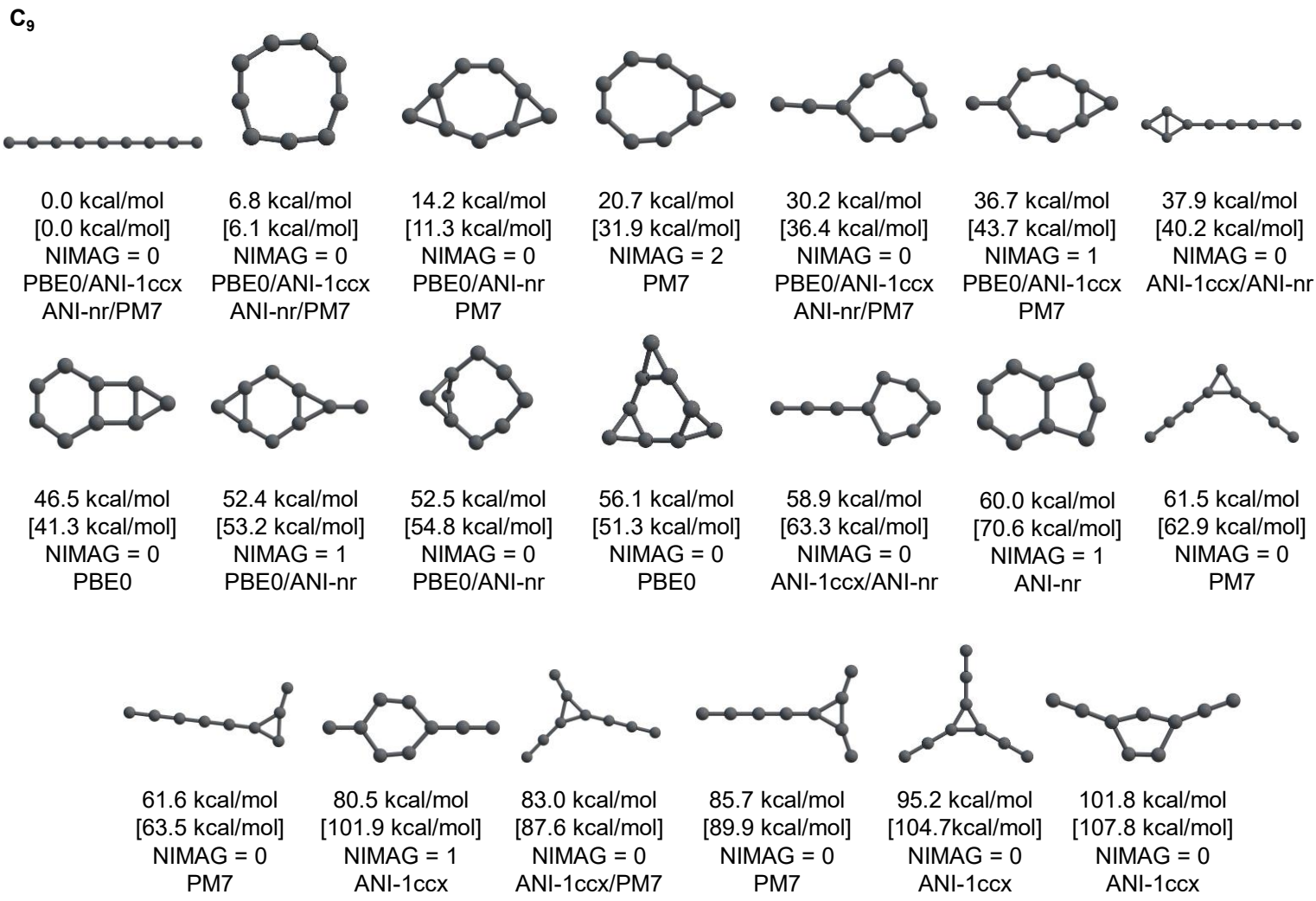

Figure S10. Optimized at PBE0/Def2-TZVPP level of theory geometries of lowest isomers of C_9. The geometries obtained via reoptimization of ten initial guessed structures obtained by PBE0/def2-SVP, PM7, ANI-nr, and ANI-1ccx methods. The relative energies are given at CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level of theory. Relative energies in square brackets are calculated at PBE0/def2-TZVPP level. Number if imaginary frequencies (NIMAG) is given. Under each structure the method that provided the initial guess geometry is given.

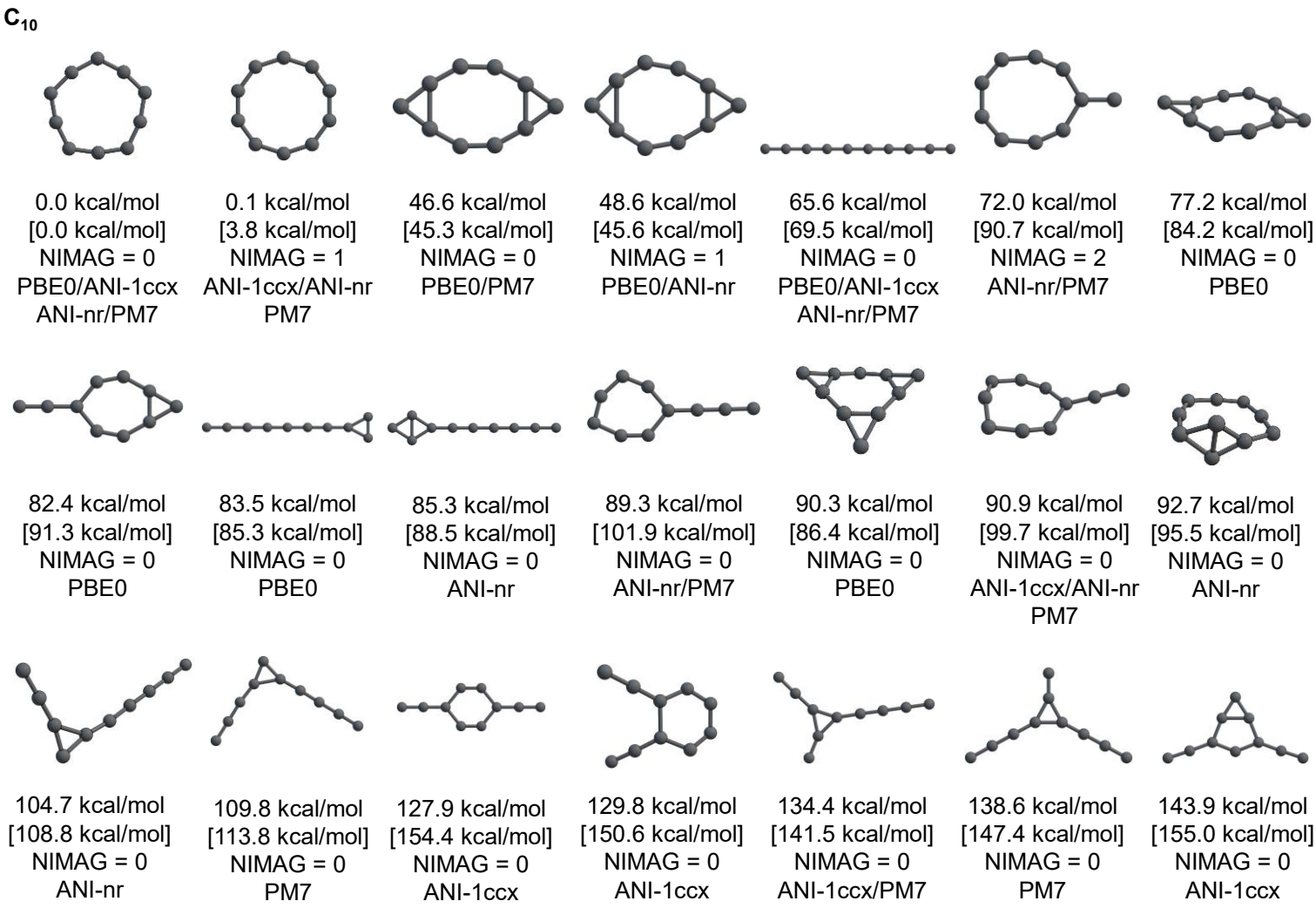

Figure S11. Optimized at PBE0/Def2-TZVPP level of theory geometries of lowest isomers of C_{10}. The geometries obtained via reoptimization of ten initial guessed structures obtained by PBE0/def2-SVP, PM7, ANI-nr, and ANI-1ccx methods. The relative energies are given at CCSD(T)/def2-TZVPP//PBE0/def2-TZVPP level of theory. Relative energies in square brackets are calculated at PBE0/def2-TZVPP level. Number if imaginary frequencies (NIMAG) is given. Under each structure the method that provided the initial guess geometry is given.

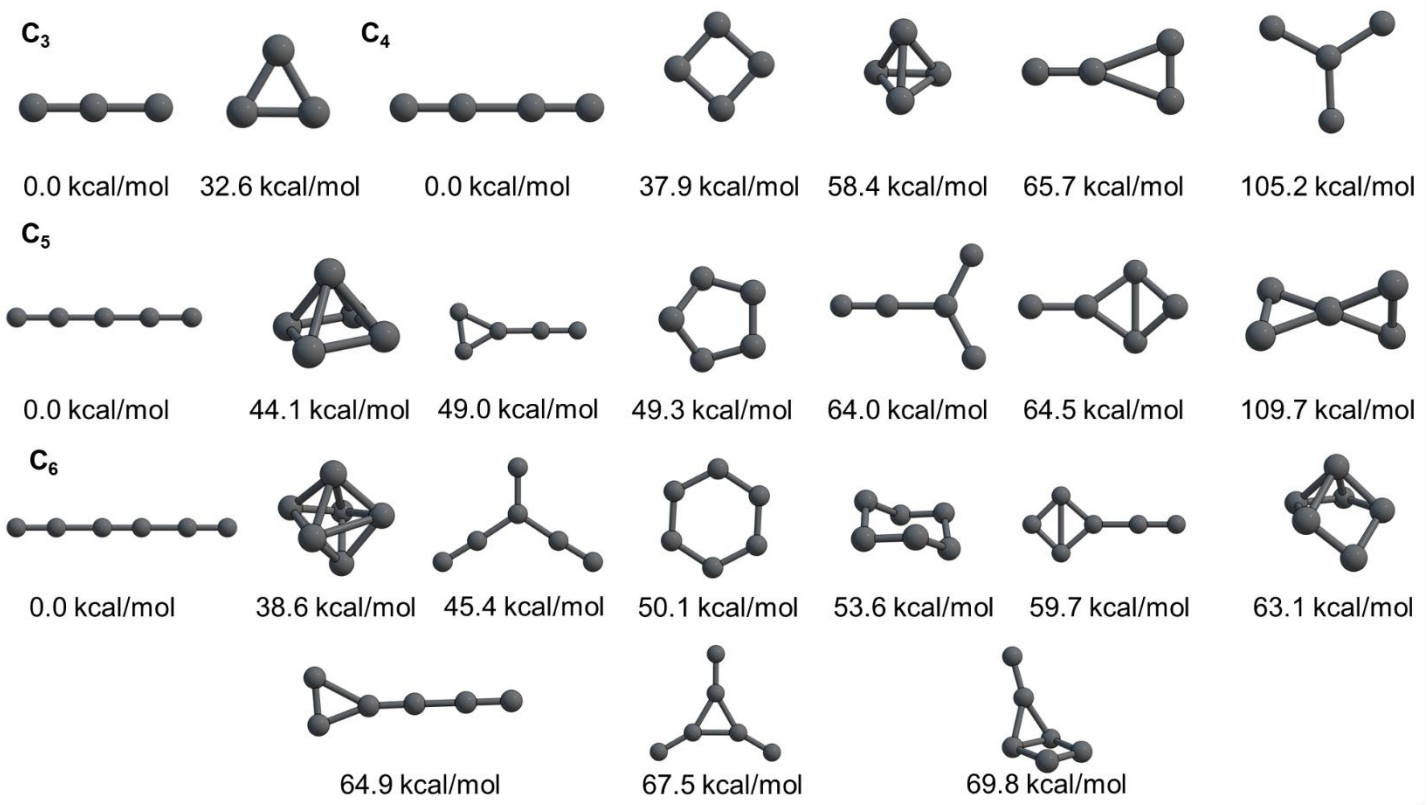

Figure S12. The lowest connected isomers of C_n (n = 3-6) clusters obtained via ANI-1ccx method.

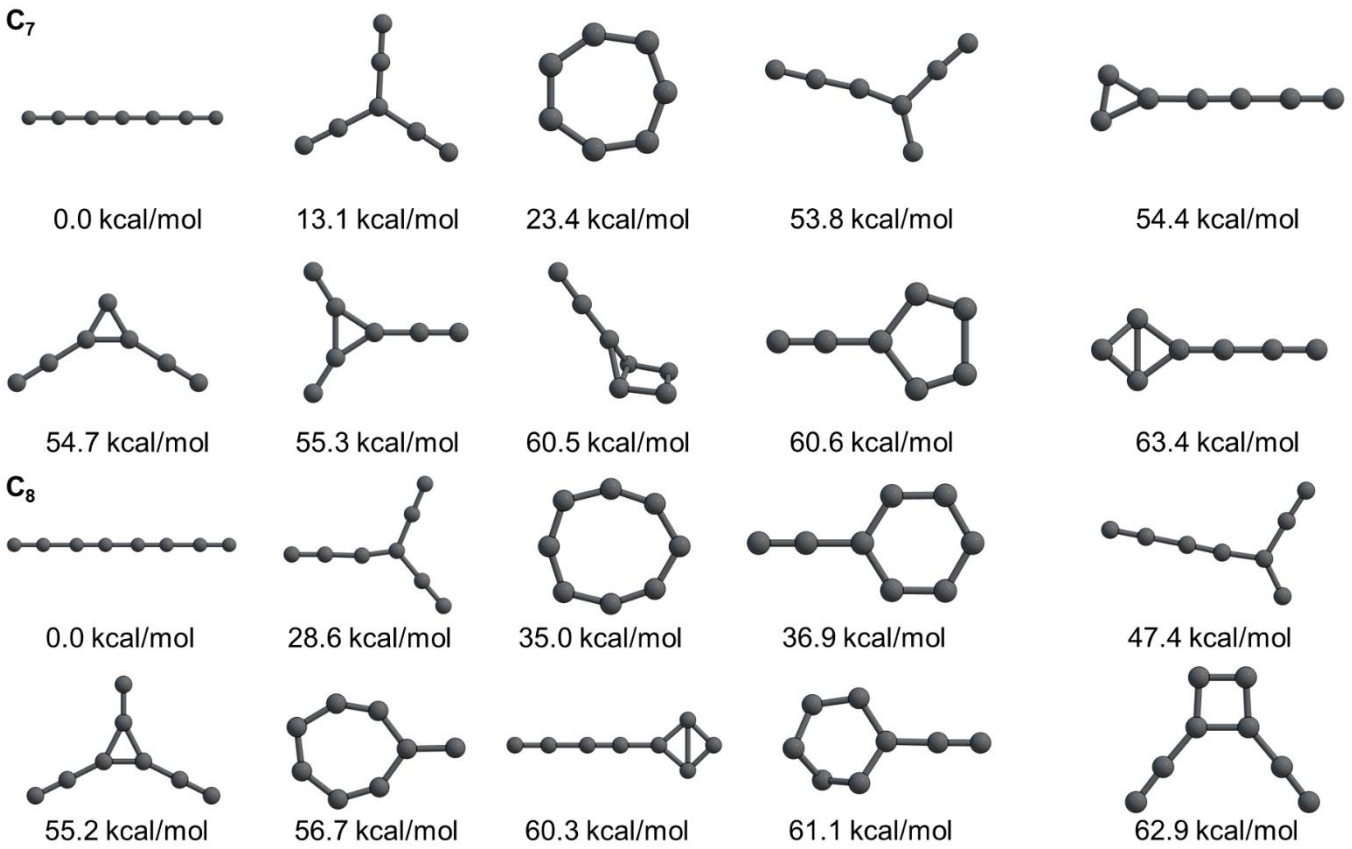

Figure S13. The lowest connected isomers of C_n (n = 7-8) clusters obtained via ANI-1ccx method.

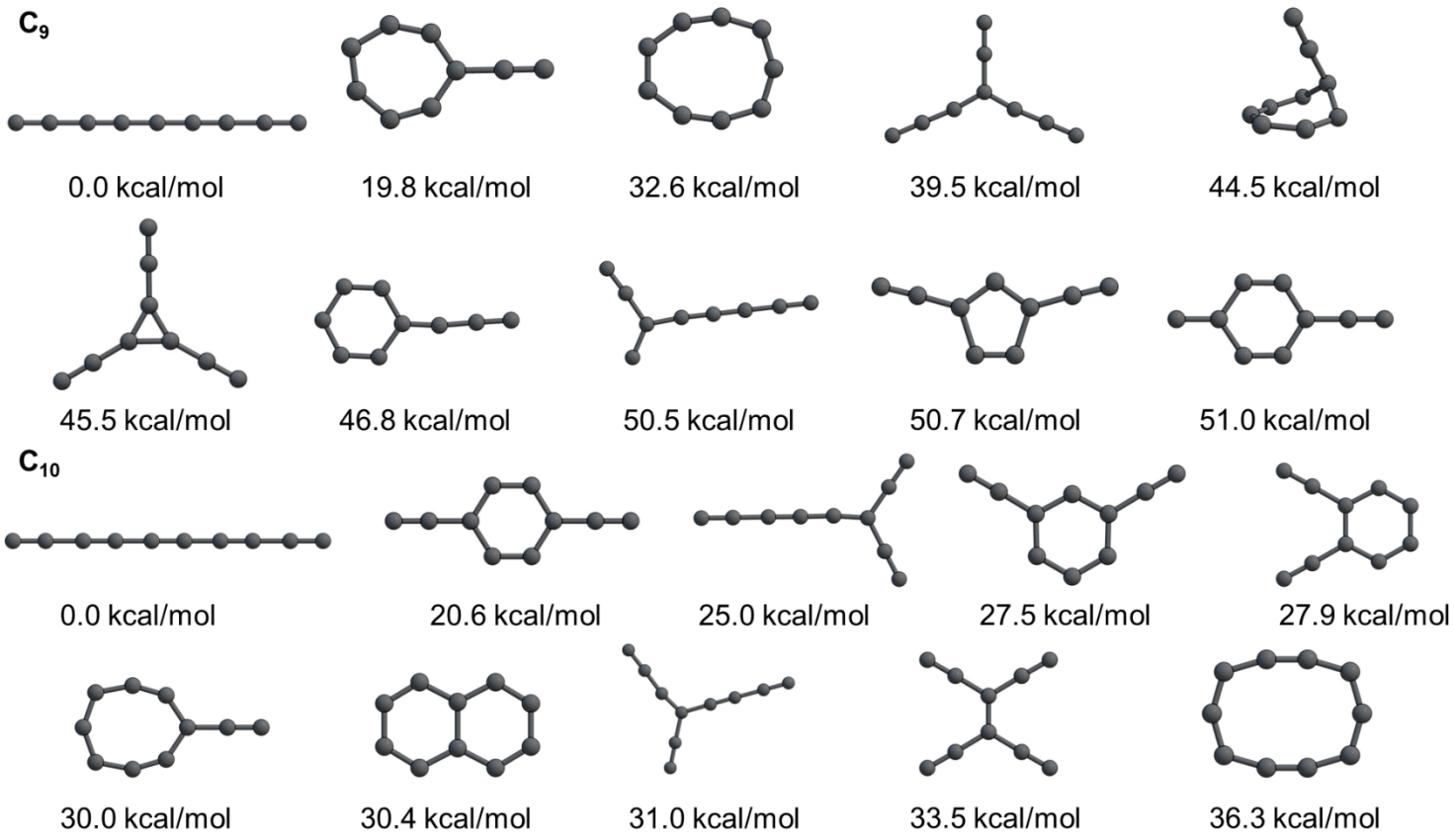

Figure S14. The lowest connected isomers of C_n (n = 9-10) clusters obtained via ANI-1ccx method.

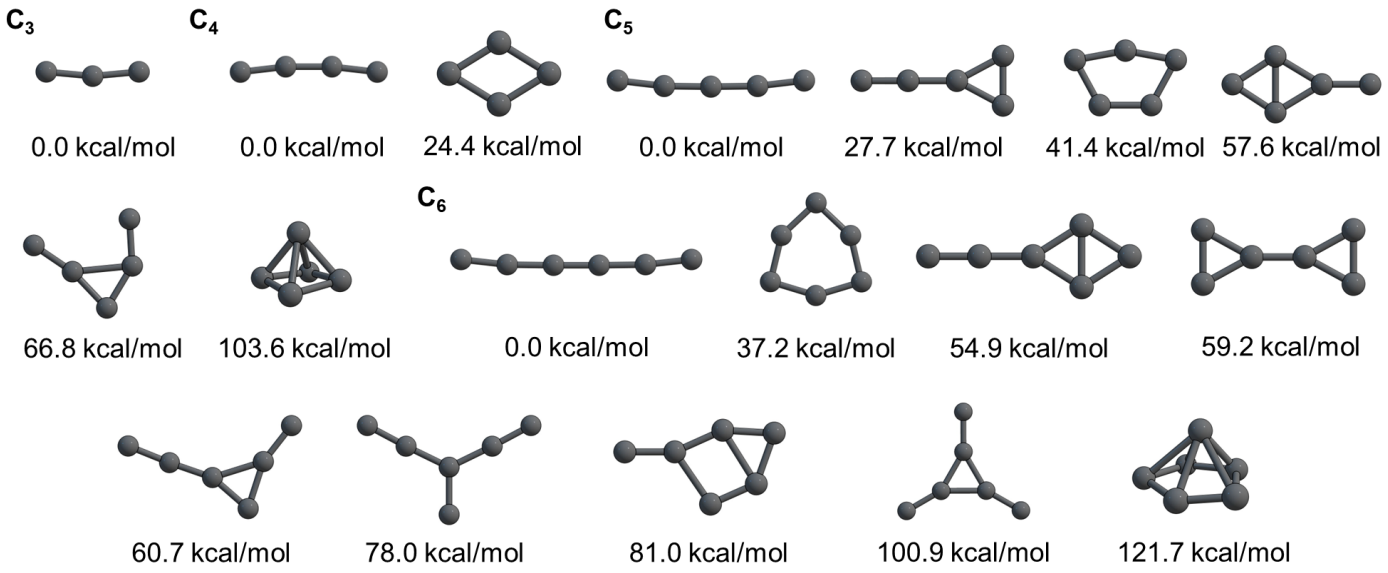

Figure S15. The lowest connected isomers of C_n (n = 3-6) clusters obtained via ANI-nr method.

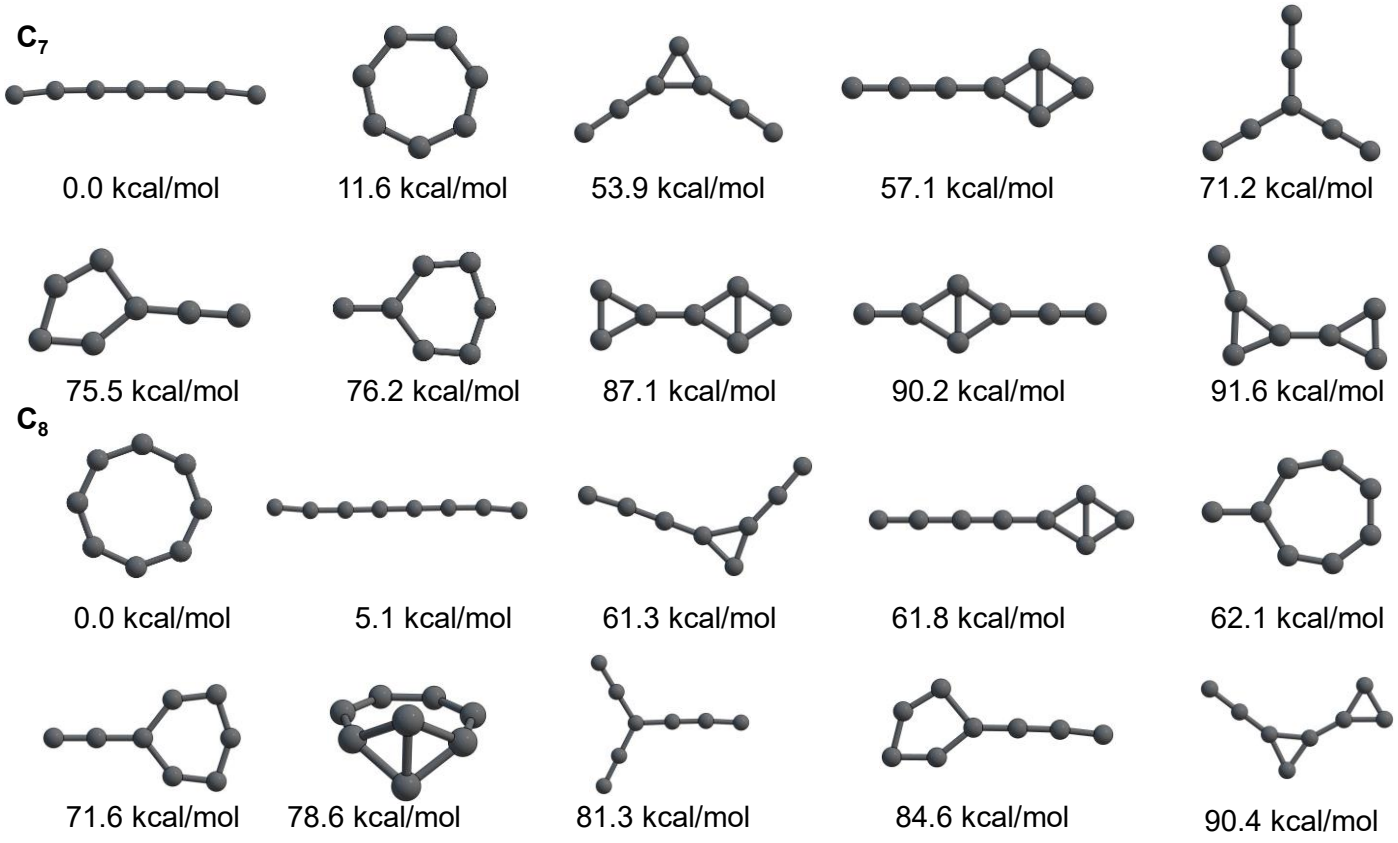

Figure S16. The lowest connected isomers of C_n (n = 7-8) clusters obtained via ANI-nr method.

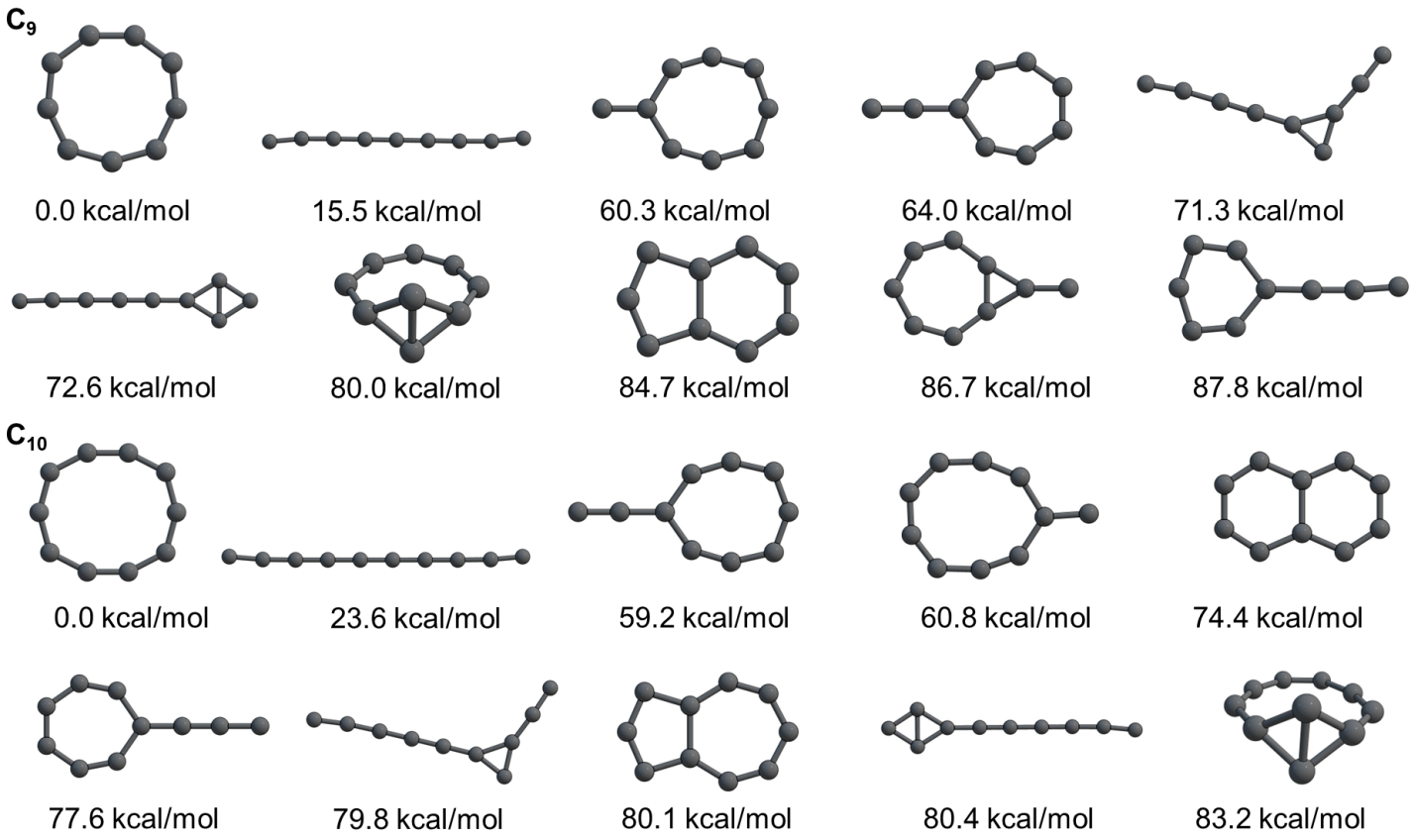

Figure S17. The lowest connected isomers of C_n (n = 9-10) clusters obtained via ANI-nr method.

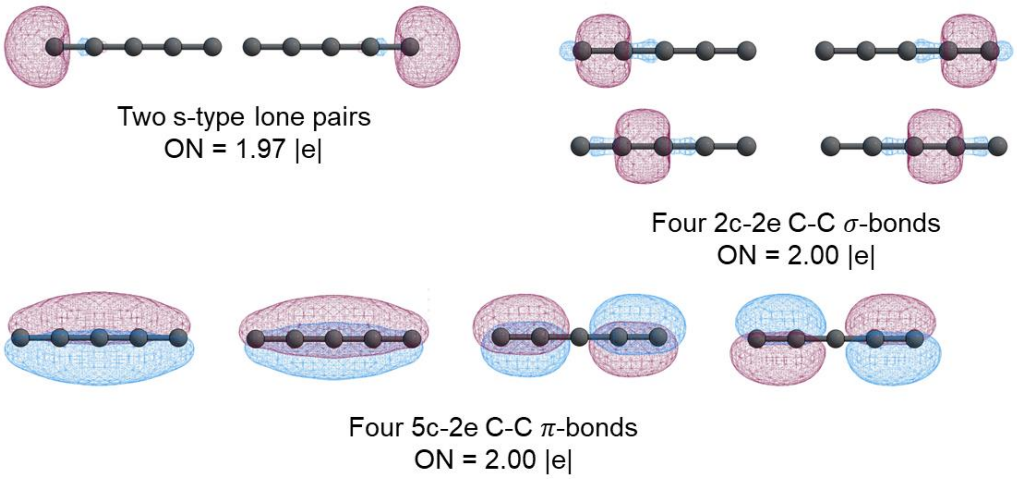

Figure S18. Chemical bonding pattern of the linear isomer of C_5 cluster obtained from AdNDP analysis.

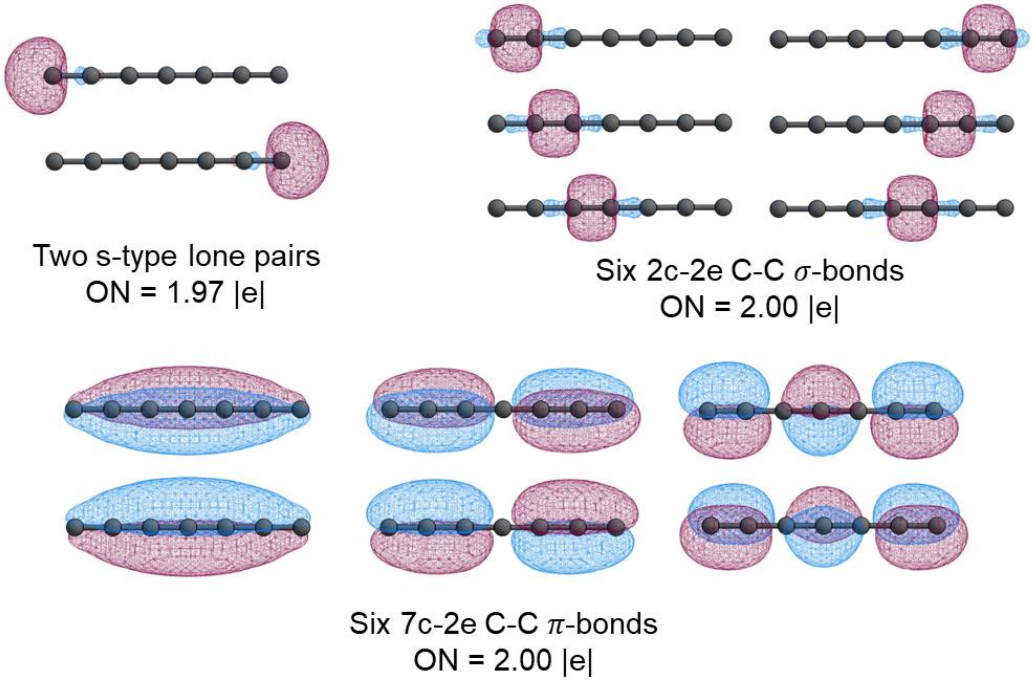

Figure S19. Chemical bonding pattern of the linear isomer of C_7 cluster obtained from AdNDP analysis.

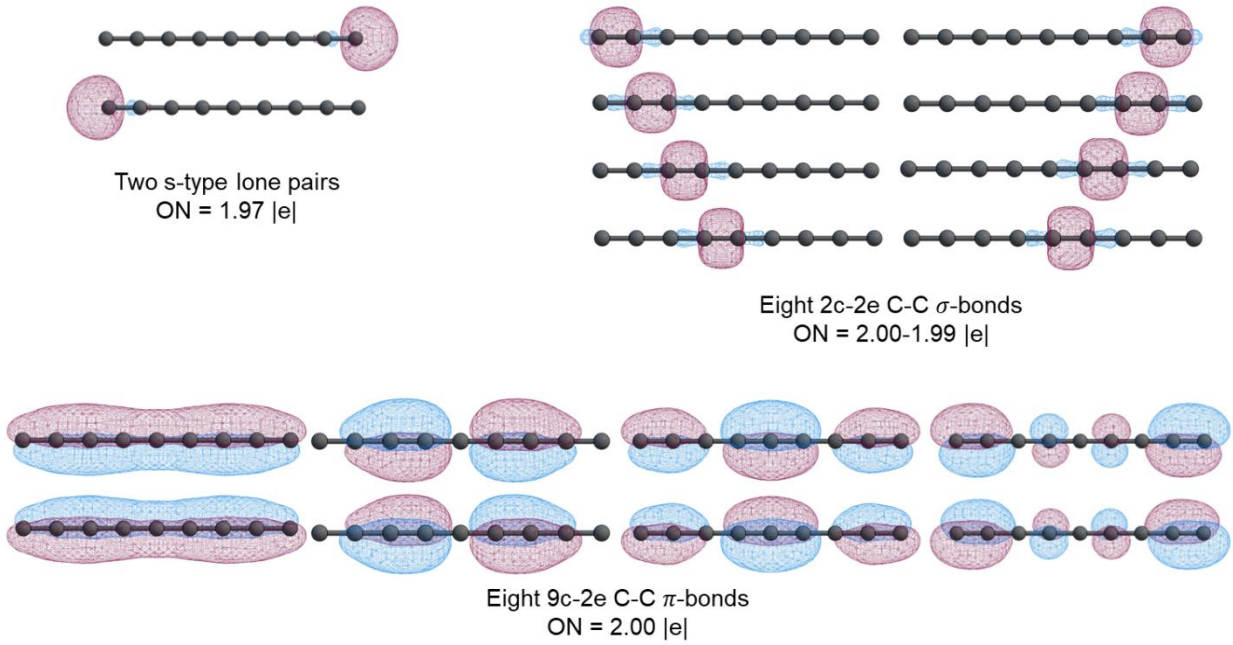

Figure S20. Chemical bonding pattern of the linear isomer of C_9 cluster obtained from AdNDP analysis.

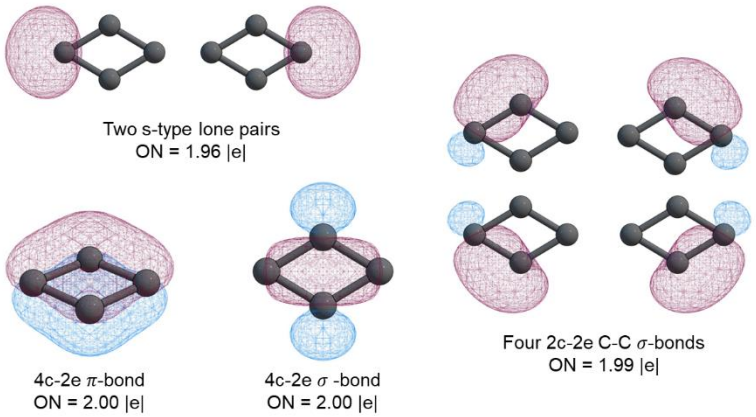

Figure S21. Chemical bonding pattern of the cyclic isomer of C_4 cluster obtained from AdNDP analysis.

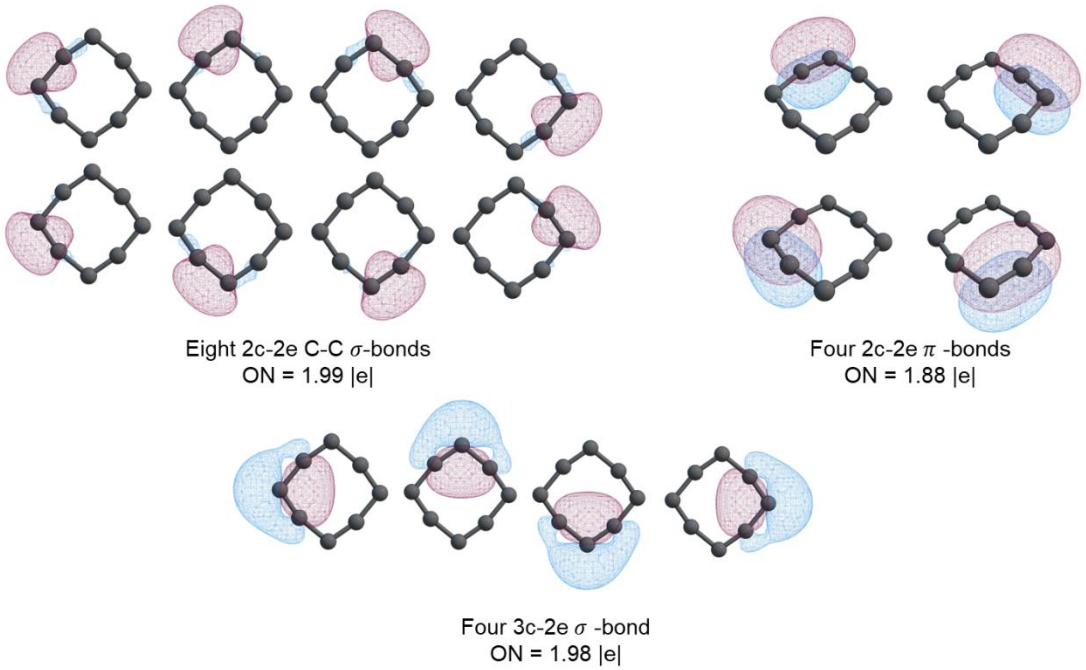

Figure S22. Chemical bonding pattern of the cyclic isomer of C_8 cluster obtained from AdNDP analysis.

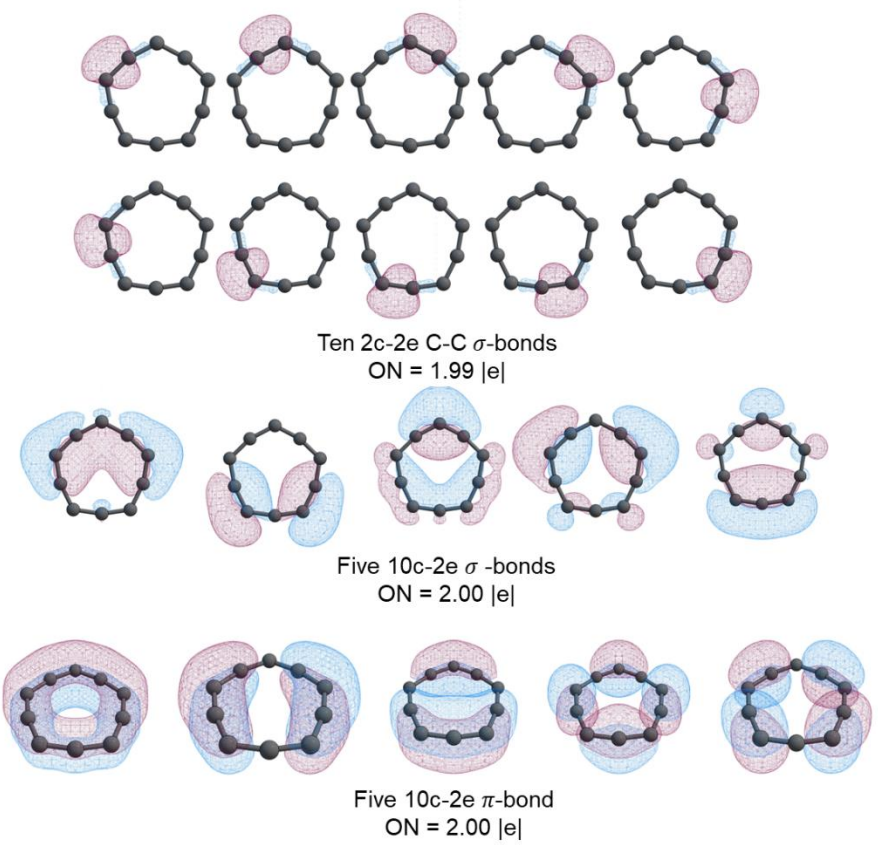

Figure S23. Chemical bonding pattern of the cyclic isomer of C_{10} cluster obtained from AdNDP analysis.

Supplementary Tables

Table S1. Absolute [a.u.] and relative [kcal/mol] energies for linear and cyclic singlet-state isomers obtained at DLPNO-CCSD(T) level of theory with three-point extrapolation to CBS.

Stoichiometry	Linear isomer	Cyclic isomer	|Relative energy|
C_3	-113.8760004	-113.8366586	24.7
C_4	-151.8331203	-151.850678	11.0
C_5	-189.9099439	-189.824336	53.7
C_6	-227.8820169	-227.915769	21.2
C_7	-265.9425417	-265.925487	10.7
C_8	-303.923935	-303.947118	14.5
C_9	-341.9755858	-341.965302	6.5
C_{10}	-379.9632593	-380.078646	72.4

Table S2. Relative [kcal/mol] energies including ZPE corrections for linear and cyclic isomers at different spin-states obtained at PBE0/Def2-TZVPP level of theory.

Stoichiometry	Cyclic isomer (S=0)	Linear isomer (S=0)	Linear isomer (S=1)
C_4	7.1	20.6	0.0
C_6	0.0	21.1	5.2
C_8	6.7	13.0	0.0
C_{10}	0.0	69.5	58.4