Supporting Information for:

Performance of Localized-Orbital Coupled Cluster Approaches for the Conformational Energies of Longer n-alkane Chains

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**Table S1:** Performance of RI-MP2 and RI-MP2-F12 methods with different basis set size for the conformer energies of $n$-dodecane ($C_nH_{2n+2}$, $n=12$). All the results are in kcal/mol unit.

| # Conf. | New Ref.[a] | RI-MP2-F12 | RI-MP2 |
|-------|-------------|------------|---------|
|       |             | VDZ-F12    | VTZ-F12  | V[T,Q]Z-F12 | def2-TZVPP | def2-QZVPP | def2-[T,Q]ZVPP | AVTZ | AVQZ | AV{T,Q}Z | AV{Q,5}Z |
| 1     | 1.82        | 1.62       | 1.61     | 1.61       | 1.60        | 1.48       | 1.56       | 1.56       | 1.62       |
| 2     | 2.05        | 1.63       | 1.62     | 1.61       | 1.60        | 1.29       | 1.52       | 1.73       | 1.22       | 1.49       | 1.56       | 1.75       | 1.64       |
| 3     | 2.49        | 2.17       | 2.16     | 2.16       | 2.15        | 1.85       | 2.06       | 2.26       | 1.82       | 2.06       | 2.11       | 2.28       | 2.18       |
| 4     | 3.16        | 2.70       | 2.71     | 2.71       | 2.70        | 2.23       | 2.56       | 2.86       | 1.95       | 2.45       | 2.61       | 2.92       | 2.79       |
| 5     | 3.66        | 3.49       | 3.50     | 3.50       | 3.49        | 3.25       | 3.42       | 3.59       | 3.15       | 3.39       | 3.46       | 3.61       | 3.53       |
| 6     | 3.88        | 3.58       | 3.58     | 3.59       | 3.58        | 3.23       | 3.47       | 3.70       | 3.08       | 3.41       | 3.52       | 3.72       | 3.65       |
| 7     | 4.16        | 3.89       | 3.89     | 3.89       | 3.88        | 3.56       | 3.79       | 4.00       | 3.47       | 3.76       | 3.83       | 4.03       | 3.92       |
| 8     | 4.31        | 3.90       | 3.90     | 3.90       | 3.89        | 3.44       | 3.75       | 4.03       | 3.16       | 3.62       | 3.79       | 4.06       | 3.99       |
| 9     | 4.89        | 4.59       | 4.60     | 4.60       | 4.59        | 4.23       | 4.48       | 4.72       | 4.13       | 4.45       | 4.54       | 4.76       | 4.63       |
| 10    | 5.45        | 5.11       | 5.12     | 5.13       | 5.11        | 4.65       | 4.98       | 5.29       | 4.41       | 4.88       | 5.03       | 5.32       | 5.20       |
| 11    | 5.99        | 5.63       | 5.64     | 5.64       | 5.63        | 5.23       | 5.51       | 5.78       | 4.98       | 5.40       | 5.54       | 5.79       | 5.72       |
| 12    | 6.56        | 6.28       | 6.28     | 6.28       | 6.27        | 5.97       | 6.19       | 6.39       | 5.83       | 6.12       | 6.22       | 6.40       | 6.33       |

| MAD (kcal/mol) | ref | 0.32 | 0.32 | 0.32 | 0.33 | 0.67 | 0.43 | 0.20 | 0.82 | 0.49 | 0.39 | 0.18 | 0.27 |
| RMSD (kcal/mol) | 0.33 | 0.33 | 0.33 | 0.34 | 0.69 | 0.44 | 0.21 | 0.85 | 0.50 | 0.40 | 0.19 | 0.28 |
| MSD (kcal/mol)  | -0.32 | -0.32 | -0.32 | -0.33 | -0.67 | -0.43 | -0.20 | -0.82 | -0.49 | -0.39 | -0.18 | -0.27 |

| MAD (kcal/mol) | ref | 0.34 | 0.10 | 0.13 | 0.49 | 0.16 | 0.06 | 0.15 | 0.06 |
| RMSD (kcal/mol) | 0.35 | 0.10 | 0.13 | 0.52 | 0.17 | 0.06 | 0.16 | 0.07 |
| MSD (kcal/mol)  | -0.34 | -0.10 | 0.13 | -0.49 | -0.16 | -0.06 | 0.15 | 0.06 |

[a] MP2-F12/V[T,Q]Z-F13 + [CCSD(F12*)-MP2-F12]/cc-pVTZ-F12 + [DF-CCSD(T)-DF-CCSD]/AV[T,D]Z
Table S2: Performance of six HLCs relative to canonical [DF-CCSD(T) - DF-MP2] with AVTZ throughout. Total [CCSD(T)-MP2] contributions has been divided into [CCSD-MP2] and (T) parts for better understanding of error compensation in different localized orbital methods. All the results are in kcal/mol unit.

| # Conf. | [DF-CCSD(T) - DF-MP2] | HLC6 | HLC7 | HLC8 | HLC3 | HLC15 | HLC16 | [DLPNO-CCSD(T) - LMP2]/TightPNO |
|---------|------------------------|------|------|------|------|-------|-------|-------------------------------|
| 1       | 0.48                   | 0.46 | 0.46 | 0.46 | 0.50 | 0.45  | 0.48  | 0.52                          |
| 2       | 0.97                   | 0.94 | 0.93 | 0.92 | 0.99 | 0.89  | 0.93  | 1.01                          |
| 3       | 0.81                   | 0.77 | 0.77 | 0.76 | 0.83 | 0.75  | 0.79  | 0.89                          |
| 4       | 1.28                   | 1.24 | 1.21 | 1.21 | 1.30 | 1.15  | 1.20  | 1.20                          |
| 5       | 0.58                   | 0.56 | 0.55 | 0.55 | 0.60 | 0.53  | 0.56  | 0.60                          |
| 6       | 0.91                   | 0.88 | 0.86 | 0.85 | 0.92 | 0.82  | 0.86  | 0.92                          |
| 7       | 0.79                   | 0.75 | 0.75 | 0.75 | 0.81 | 0.72  | 0.76  | 0.82                          |
| 8       | 1.26                   | 1.23 | 1.19 | 1.19 | 1.29 | 1.15  | 1.18  | 1.20                          |
| 9       | 0.93                   | 0.90 | 0.88 | 0.87 | 0.95 | 0.84  | 0.89  | 0.95                          |
| 10      | 1.15                   | 1.11 | 1.08 | 1.08 | 1.17 | 1.03  | 1.08  | 1.12                          |
| 11      | 1.17                   | 1.14 | 1.11 | 1.10 | 1.20 | 1.05  | 1.09  | 1.16                          |
| 12      | 0.93                   | 0.89 | 0.88 | 0.88 | 0.96 | 0.85  | 0.89  | 0.97                          |

| MAD     | 0.034  | 0.050  | 0.053  | 0.021  | 0.087  | 0.047  | 0.037  |
| RMSD    | 0.035  | 0.052  | 0.055  | 0.022  | 0.091  | 0.053  | 0.043  |
| MSD     | -0.034 | -0.050 | -0.053 | 0.021  | -0.087 | -0.047 | 0.007  |

| # Conf. | [DF-CCSD(T) - DF-MP2] | HLC6 | HLC7 | HLC8 | HLC3 | HLC15 | HLC16 | [DLPNO-CCSD(T) - LMP2]/TightPNO |
|---------|------------------------|------|------|------|------|-------|-------|-------------------------------|
| 1       | -0.25                  | -0.26| -0.23| -0.24| -0.24| -0.21 | -0.23 | -0.26                         |
| 2       | -0.49                  | -0.52| -0.46| -0.47| -0.48| -0.44 | -0.45 | -0.49                         |
| 3       | -0.44                  | -0.44| -0.41| -0.41| -0.43| -0.39 | -0.40 | -0.44                         |
| 4       | -0.75                  | -0.82| -0.71| -0.70| -0.73| -0.67 | -0.69 | -0.70                         |
| 5       | -0.39                  | -0.42| -0.38| -0.38| -0.38| -0.35 | -0.36 | -0.39                         |
| 6       | -0.57                  | -0.61| -0.54| -0.54| -0.56| -0.51 | -0.52 | -0.55                         |
| 7       | -0.49                  | -0.51| -0.47| -0.46| -0.48| -0.43 | -0.44 | -0.48                         |
| 8       | -0.78                  | -0.84| -0.73| -0.72| -0.75| -0.69 | -0.71 | -0.72                         |
| 9       | -0.60                  | -0.63| -0.57| -0.57| -0.59| -0.53 | -0.55 | -0.58                         |
| 10      | -0.77                  | -0.81| -0.72| -0.72| -0.74| -0.68 | -0.70 | -0.73                         |
| 11      | -0.76                  | -0.82| -0.72| -0.72| -0.74| -0.67 | -0.69 | -0.71                         |
| 12      | -0.62                  | -0.64| -0.60| -0.60| -0.61| -0.55 | -0.57 | -0.60                         |

| MAD     | 0.034  | 0.031  | 0.033  | 0.017  | 0.067  | 0.051  | 0.025  |
| RMSD    | 0.039  | 0.033  | 0.036  | 0.019  | 0.070  | 0.053  | 0.032  |
| MSD     | -0.034 | -0.031 | -0.033 | 0.017  | 0.067  | 0.051  | 0.022  |

| # Conf. | [DF-CCSD(T) - DF-MP2] | HLC6 | HLC7 | HLC8 | HLC3 | HLC15 | HLC16 | [DLPNO-CCSD(T) - LMP2]/TightPNO |
|---------|------------------------|------|------|------|------|-------|-------|-------------------------------|
| 1       | 0.24                   | 0.20 | 0.23 | 0.22 | 0.25 | 0.23  | 0.25  | 0.26                          |
| 2       | 0.48                   | 0.42 | 0.46 | 0.46 | 0.50 | 0.46  | 0.48  | 0.52                          |
| 3       | 0.37                   | 0.33 | 0.36 | 0.35 | 0.40 | 0.36  | 0.39  | 0.45                          |
| 4       | 0.52                   | 0.42 | 0.50 | 0.51 | 0.58 | 0.49  | 0.51  | 0.51                          |
| 5       | 0.19                   | 0.13 | 0.17 | 0.17 | 0.22 | 0.18  | 0.20  | 0.21                          |
| 6       | 0.33                   | 0.27 | 0.31 | 0.32 | 0.37 | 0.32  | 0.34  | 0.38                          |
| 7       | 0.31                   | 0.24 | 0.28 | 0.28 | 0.34 | 0.29  | 0.32  | 0.33                          |
| 8       | 0.48                   | 0.39 | 0.46 | 0.47 | 0.54 | 0.46  | 0.47  | 0.48                          |
| 9       | 0.33                   | 0.27 | 0.31 | 0.31 | 0.37 | 0.31  | 0.34  | 0.37                          |
| 10      | 0.38                   | 0.30 | 0.36 | 0.36 | 0.43 | 0.35  | 0.38  | 0.39                          |
| 11      | 0.40                   | 0.31 | 0.38 | 0.38 | 0.46 | 0.38  | 0.40  | 0.44                          |
| 12      | 0.31                   | 0.25 | 0.28 | 0.28 | 0.35 | 0.30  | 0.32  | 0.37                          |

| MAD     | 0.068  | 0.019  | 0.020  | 0.038  | 0.020  | 0.009  | 0.033  |
| RMSD    | 0.070  | 0.020  | 0.021  | 0.040  | 0.022  | 0.010  | 0.038  |
| MSD     | -0.068 | -0.019 | -0.020 | 0.038  | -0.020 | 0.003  | 0.029  |
Table S3: Performance of localized orbital based high-level corrections relative to the canonical [CCSD(F12*)] − MP2-F12/[VTZ-F12 + (T)/AV{D,T}Z correction used for the reference conformer energies of n-dodecane.

| # Conformers in the ACONF12 set | MAD (kcal/mol) | RMSD (kcal/mol) | MSD (kcal/mol) |
|----------------------------------|----------------|-----------------|----------------|
|                                 | 01  | 02  | 03  | 04  | 05  | 06  | 07  | 08  | 09  | 10  | 11  | 12  |       |
| HLC1\(^a\)                     | 0.22| 0.45| 0.34| 0.46| 0.17| 0.30| 0.28| 0.42| 0.30| 0.34| 0.36| 0.29| 0.035 |
| HLC2\(^a\)                     | 0.24| 0.48| 0.37| 0.52| 0.19| 0.33| 0.31| 0.48| 0.33| 0.38| 0.40| 0.31| 0.038 |
| HLC3\(^a\)                     | 0.25| 0.51| 0.43| 0.50| 0.20| 0.36| 0.32| 0.47| 0.35| 0.37| 0.44| 0.35| 0.035 |
| HLC4\(^a\)                     | 0.27| 0.55| 0.43| 0.63| 0.25| 0.42| 0.38| 0.61| 0.43| 0.51| 0.53| 0.42| 0.050 |
| HLC5\(^a\)                     | 0.33| 0.58| 0.46| 0.58| 0.24| 0.41| 0.43| 0.58| 0.43| 0.47| 0.53| 0.44| 0.073 |
| HLC6\(^a\)                     | 0.20| 0.42| 0.33| 0.42| 0.13| 0.27| 0.24| 0.39| 0.27| 0.30| 0.31| 0.25| 0.032 |
| HLC7\(^a\)                     | 0.23| 0.46| 0.36| 0.50| 0.17| 0.31| 0.28| 0.46| 0.31| 0.36| 0.38| 0.28| 0.017 |
| HLC8\(^a\)                     | 0.22| 0.46| 0.35| 0.51| 0.17| 0.32| 0.28| 0.47| 0.31| 0.36| 0.38| 0.28| 0.016 |
| HLC9\(^a\)                     | 0.21| 0.44| 0.35| 0.45| 0.15| 0.29| 0.26| 0.43| 0.30| 0.34| 0.35| 0.28| 0.009 |
| HLC10\(^a\)                    | 0.26| 0.50| 0.40| 0.55| 0.20| 0.36| 0.32| 0.51| 0.36| 0.42| 0.44| 0.33| 0.059 |
| HLC11\(^a\)                    | 0.24| 0.48| 0.38| 0.51| 0.19| 0.33| 0.30| 0.47| 0.33| 0.38| 0.40| 0.31| 0.031 |
| HLC12\(^a\)                    | 0.27| 0.52| 0.42| 0.58| 0.23| 0.39| 0.35| 0.55| 0.39| 0.45| 0.47| 0.37| 0.088 |
| HLC13\(^a\)                    | 0.22| 0.46| 0.36| 0.47| 0.16| 0.31| 0.27| 0.45| 0.31| 0.36| 0.38| 0.30| 0.012 |
| HLC14\(^a\)                    | 0.22| 0.45| 0.36| 0.46| 0.17| 0.29| 0.28| 0.42| 0.31| 0.34| 0.36| 0.28| 0.006 |
| HLC15\(^a\)                    | 0.23| 0.46| 0.36| 0.49| 0.18| 0.32| 0.29| 0.46| 0.31| 0.35| 0.38| 0.30| 0.015 |
| HLC16\(^a\)                    | 0.25| 0.48| 0.39| 0.51| 0.20| 0.34| 0.32| 0.47| 0.34| 0.38| 0.40| 0.32| 0.038 |
| HLC17\(^a\)                    | 0.25| 0.47| 0.38| 0.50| 0.20| 0.33| 0.31| 0.47| 0.34| 0.38| 0.40| 0.33| 0.035 |
| HLC18\(^a\)                    | 0.25| 0.48| 0.39| 0.52| 0.22| 0.35| 0.33| 0.49| 0.36| 0.40| 0.42| 0.35| 0.052 |
| HLC19\(^a\)                    | 0.26| 0.48| 0.39| 0.51| 0.21| 0.34| 0.33| 0.48| 0.35| 0.39| 0.42| 0.35| 0.048 |
| HLC20\(^a\)                    | 0.26| 0.49| 0.40| 0.53| 0.23| 0.36| 0.34| 0.50| 0.37| 0.41| 0.44| 0.36| 0.062 |
| HLC21\(^a\)                    | 0.28| 0.51| 0.41| 0.56| 0.24| 0.38| 0.36| 0.53| 0.40| 0.44| 0.47| 0.40| 0.087 |
| HLC22\(^a\)                    | 0.29| 0.52| 0.43| 0.56| 0.25| 0.39| 0.37| 0.52| 0.40| 0.44| 0.46| 0.39| 0.091 |

\[DF\]CCSD(T) − RI-MP2/AVTZ
\[DLPNO-CCSD(T1) − LMP2\]/TightPNO/CPS\{6,7\}/AVTZ
\[DLPNO-CCSD(T1) − LMP2\]/VeryTightPNO/AVTZ
\[DLPNO-CCSD(T1) − LMP2\]/VeryTightPNO/AV[T,Q]Z
\[DLPNO-CCSD(T1) − LMP2\]/TightPNO/CPS\{6,7\}/AV[T,Q]Z
\[LNO-CCSD(T) − LMP2\]/Tight/AVTZ
\[LNO-CCSD(T) − LMP2\]/\texttt{vTight}/AVTZ
\[LNO-CCSD(T) − LMP2\]/Tight/AVQZ
\[LNO-CCSD(T) − LMP2\]/\texttt{vTight}/AVQZ
\[LNO-CCSD(T) − LMP2\]/Tight/AVSZ
\[LNO-CCSD(T) − LMP2\]/\texttt{vTight}/AV[T,Q]Z
\[LNO-CCSD(T) − LMP2\]/Tight/AV[T,Q]Z
\[LNO-CCSD(T) − LMP2\]/\texttt{vTight}/AVQZ
\[LNO-CCSD(T) − LMP2\]/Tight/AVQZ
\[PNO-LCCSD(T) − LMP2\]/Default/AVTZ
\[PNO-LCCSD(T) − LMP2\]/Tight/AVTZ
\[PNO-LCCSD(T) − LMP2\]/Default/AVQZ
\[PNO-LCCSD(T) − LMP2\]/Tight/AVQZ
\[PNO-LCCSD(T) − LMP2\]/Default/AV[T,Q]Z
\[PNO-LCCSD(Ts)-F12b − LMP2-F12\]/Default/VTZ-F12
\[PNO-LCCSD(Ts)-F12b − LMP2-F12\]/Tight/VTZ-F12

S4
Table S4: Conformer energies of \(n\)-dodecane, \(n\)-hexadecane, and \(n\)-icosane with three high-level corrections (HLC14, HLC8, and HLC13) using localized orbital methods. For convenience, we have retained the numbering and ordering of different conformers from ref.\(^1\); conformer energies of \(n\)-dodecane and \(n\)-hexadecane are relative to the all-trans conformer 0, while those for \(n\)-icosane are relative to the “hairpin” conformer 00.

|        | RI-MP2-F12/V\(\{T,Q\}\)Z-F12 + HLC |        | RI-MP2-F12/V\(\{T,Q\}\)Z-F12 + HLC |        | RI-MP2-F12/V\(\{T,Q\}\)Z-F12 + HLC |
|--------|--------------------------------------|--------|--------------------------------------|--------|--------------------------------------|
|        | HLC14\(^{(a)}\) HLC8\(^{(b)}\) HLC13\(^{(c)}\) | #       | HLC14\(^{(a)}\) HLC8\(^{(b)}\) HLC13\(^{(c)}\) | #       | HLC14\(^{(a)}\) HLC8\(^{(b)}\) HLC13\(^{(c)}\) |
| 1      | 1.82 1.82 1.79                         | 0       | -0.49 -0.39 -0.49                    | 0       | 2.20 2.06 2.19                      |
| 2      | 2.06 2.06 2.01                         | 1       | 2.15 2.19 2.10                       | 1       | 4.15 4.10 4.07                      |
| 3      | 2.51 2.50 2.47                         | 3       | 2.54 2.57 2.47                       | 5       | 4.81 4.67 4.75                      |
| 4      | 3.16 3.21 3.10                         | 4       | 2.68 2.68 2.63                       | 6       | 4.99 4.87 4.91                      |
| 5      | 3.65 3.66 3.61                         | 2       | 2.94 2.98 2.87                       | 7       | 5.27 5.14 5.21                      |
| 6      | 3.87 3.89 3.83                         | 6       | 3.24 3.23 3.14                       | 3       | 4.85 4.81 4.74                      |
| 7      | 4.16 4.16 4.11                         | 7       | 3.28 3.29 3.21                       | 11      | 5.60 5.47 5.52                      |
| 8      | 4.31 4.36 4.25                         | 5       | 3.34 3.35 3.25                       | 10      | 5.58 5.46 5.50                      |
| 9      | 4.90 4.90 4.84                         | 8       | 3.68 3.68 3.62                       | 4       | 5.31 5.26 5.23                      |
| 10     | 5.45 5.48 5.40                         | 9       | 3.98 3.99 3.93                       | 12      | 5.74 5.61 5.69                      |
| 11     | 5.99 6.01 5.92                         | 10      | 4.08 4.12 4.03                       | 8       | 5.28 5.27 5.21                      |
| 12     | 6.55 6.56 6.50                         | 11      | 4.35 4.36 4.31                       | 2       | 5.05 5.11 4.95                      |
| 13     | 4.54 4.54 4.47                         | 9       | 5.77 5.65 5.67                       | 16      | 6.01 5.89 5.91                      |
| 14     | 4.95 4.95 4.89                         | 16      | 6.01 5.89 5.91                       | 16      | 6.12 5.99 6.03                      |
| 15     | 5.02 5.00 4.95                         | 13      | 6.12 5.99 6.03                       | 17      | 6.33 6.24 6.24                      |
| 16     | 5.84 5.94 5.71                         | 17      | 6.33 6.24 6.24                       | 15      | 6.52 6.39 6.41                      |
| 17     | 6.11 6.15 6.02                         | 15      | 6.52 6.39 6.41                       | 19      | 6.65 6.52 6.56                      |
| 18     | 6.74 6.73 6.63                         | 14      | 6.38 6.36 6.28                       | 14      | 6.74 6.73 6.63                      |
| 19     | 7.94 7.97 7.81                         | 20      | 7.94 7.97 7.81                       |

\(^{(a)}\)HLC14 = [LNO-CCSD(T) − LMP2]/vTight/AV\{Q,5\}Z

\(^{(b)}\)HLC8 = [LNO-CCSD(T) − LMP2]/vvTight/AVTZ

\(^{(c)}\)HLC13 = [LNO-CCSD(T) − LMP2]/Tight/AV\{T,Q\}Z
Table S5: ACONF16 conformer energies relative to the 00 (hairpin) conformer.

| # Conf. ACONF16 | MP2-F12/V{T,Q}Z-F12+HLC | HLC14<sup>(a)</sup> | HLC8<sup>(b)</sup> | HLC13<sup>(c)</sup> |
|----------------|--------------------------|---------------------|------------------|------------------|
| 0              |                          | 0.49                | 0.39             | 0.49             |
| 1              |                          | 2.64                | 2.58             | 2.58             |
| 3              |                          | 3.02                | 2.96             | 2.96             |
| 4              |                          | 3.16                | 3.07             | 3.12             |
| 2              |                          | 3.43                | 3.38             | 3.36             |
| 6              |                          | 3.72                | 3.62             | 3.63             |
| 7              |                          | 3.77                | 3.69             | 3.69             |
| 5              |                          | 3.83                | 3.75             | 3.73             |
| 8              |                          | 4.17                | 4.08             | 4.11             |
| 9              |                          | 4.47                | 4.39             | 4.41             |
| 10             |                          | 4.57                | 4.51             | 4.52             |
| 11             |                          | 4.84                | 4.75             | 4.79             |
| 12             |                          | 5.03                | 4.94             | 4.96             |
| 14             |                          | 5.43                | 5.34             | 5.38             |
| 13             |                          | 5.51                | 5.40             | 5.44             |
| 15             |                          | 6.33                | 6.33             | 6.19             |
| 16             |                          | 6.59                | 6.55             | 6.51             |

<sup>(a) HLC14 = [LNO-CCSD(T) − LMP2]/vTight/AV{Q,5}Z</sup>  
<sup>(b) HLC8 = [LNO-CCSD(T) − LMP2]/vvTight/AVTZ</sup>  
<sup>(c) HLC13 = [LNO-CCSD(T) − LMP2]/Tight/AV{T,Q}Z</sup>
| Method Details | Composite methods | $c_i$ | MAD (kcal/mol) | MSD (kcal/mol) | RMSD (kcal/mol) |
|----------------|-------------------|------|----------------|---------------|-----------------|
| LNO-CCSD(T)    | Normal [T,Q] + c[TightPNO – Normal]/T | 0.93 | 0.23 0.26 0.28 0.18 | 0.09 0.26 |
|                | Normal [Q,5] + c[TightPNO – Normal]/T | 1.09 | 0.18 0.15 0.28 0.12 | 0.17 0.21 |
|                | Tight [T,Q] + c[vTight – Tight]/T | 0.79 | 0.23 0.21 0.25 0.22 | 0.05 0.25 |
|                | Tight [T,Q] + c[TightPNO – Tight]/T | 0.72 | 0.23 0.21 0.24 0.23 | 0.04 0.25 |
|                | Tight [Q,5] + c[vTight – Tight]/T | 1.26 | 0.12 0.11 0.13 0.12 | 0.03 0.13 |
|                | Tight [Q,5] + c[vTight – Tight]/Q | 1.14 | 0.08 0.05 0.08 0.09 | 0.00 0.09 |
|                | Tight [Q,5] + c[TightPNO – Tight]/T | 1.11 | 0.12 0.11 0.11 0.13 | 0.02 0.13 |
|                | vTight [T,Q] + c[vTight – Tight]/T | 0.77 | 0.26 0.23 0.30 0.24 | 0.08 0.28 |
|                | vTight [Q,5] + c[vTight – Tight]/T + c[vTight – Tight]/Q | \(c_i=2.45\) | 0.08 0.05 0.05 0.12 | -0.02 0.10 |
| PNO-LCCSD(T)   | Default [T,Q] + c[TightPNO – Tight]/T | 0.39 | 0.14 0.14 0.18 0.10 | 0.10 0.15 |
|                | Tight [T,Q] + c[TightPNO – Tight]/T | 0.30 | 0.17 0.19 0.25 0.10 | 0.12 0.19 |
|                | Tight [T,Q] + c[TightPNO – Tight]/Q | 0.66 | 0.19 0.21 0.27 0.11 | 0.13 0.21 |
| DLPNO-CCSD(T)  | NormalPNO [T,Q] + c[TightPNO – NormalPNO]/T | 0.90 | 0.13 0.14 0.20 0.07 | 0.13 0.15 |
|                | NormalPNO [T,Q] + c[TightPNO – NormalPNO]/T | 0.93 | 0.14 0.11 0.16 0.14 | 0.13 0.15 |
|                | TightPNO [T,Q] + c[TightPNO – TightPNO]/T | 1.02 | 0.25 0.23 0.31 0.20 | 0.10 0.27 |
|                | TightPNO [T,Q] + c[TightPNO – TightPNO]/Q | 0.05 | 0.14 0.18 0.24 0.05 | 0.11 0.17 |
|                | (T)TightPNO/Q + c[(T)TightPNO/Q – TightPNO/Q] | \(c_i=0.61\) | 0.10 0.12 0.16 0.04 | 0.09 0.12 |

Coefficients ($c_i$) are taken from the “Raw” category of Ref. 7.

**Table S6:** Performance of the composite LNO-CCSD(T), PNO-LCCSD(T), DLPNO-CCSD(T), and DLPNO-CCSD(T) methods with respect to the revised ACONFL reference data. Heatmapping is from red (worst) via yellow to green (best). [a]
| DL PNO-CCSD(T0) | Normal PNO{T,Q} + c1[Tight PNO - Normal PNO]/T | Normal PNO{T,Q} + c1[Tight PNO/CPS{6,7} - Normal PNO]/T | Tight PNO{T,Q} + c1[VeryTight PNO - Tight PNO]/T | Tight PNO{T,Q}/CPS{6,7} + c1[Tight PNO/CPS{6,7} - Normal PNO]/T | (T0)Tight PNO/Q + c1[(T0)Tight PNO/Q - (T0)Tight PNO]/T] + c2[(T0)Tight PNO/T] - c2| |
|------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|-------------------------------------------|---------------------------------------------|---|
|                  | 0.32                                        | 0.06                                        | 0.01                                        | 0.05                                      | 0.10                                        | 0.00 | 0.01 |
|                  | -1.28                                       | -0.02                                       | 0.05                                        | 0.26                                      | 0.08                                        | 0.00 | 0.00 |
|                  | -0.99                                       | 0.05                                        | 0.08                                        | 0.12                                      | 0.27                                        | 0.00 | 0.00 |
|                  | c1=1.25, c2=16.81                          | 0.03                                        | 0.03                                        | 0.03                                      | 0.04                                        | 0.00 | 0.00 |

[a] The expression CPS{X,Y} refers to the extrapolation of $T_{cut}$PNO to the complete PNO space limit using $T_{cut}$PNO=$10^{-X}$ and $10^{-Y}$, where Y=X+1
Table S7: Performance of pure and composite LNO-CCSD(T), PNO-LCCSD(T), and DLPNO-CCSD(T\(_1\)) methods with respect to the revised reference conformer energies of \(n\)-hexadecane and \(n\)-icosane using HLC8. Heatmapping is from red (worst) via yellow to green (best).

| Method Details       | Basis set | MAD (kcal/mol) | MSD (kcal/mol) | RMSD (kcal/mol) |
|----------------------|-----------|----------------|----------------|-----------------|
|                      | ACONFL    | ACONF12        | ACONF16        | ACONF20         |                  |
| LNO-CCSD(T) Normal   | AVTZ      | 1.00           | 0.77           | 1.00            | -0.11           | 1.10            |
|                      | AVQZ      | 0.41           | 0.29           | 0.41            | 0.47            | -0.03           | 0.45            |
|                      | AVSZ      | 0.30           | 0.21           | 0.24            | 0.40            | 0.03            | 0.34            |
|                      | AV\{T,Q\}Z | 0.05           | 0.03           | 0.04            | 0.07            | 0.02            | 0.07            |
|                      | AV\{Q,5\}Z | 0.21           | 0.14           | 0.11            | 0.34            | 0.09            | 0.26            |
| LNO-CCSD(T) Tight    | AVTZ      | 0.85           | 0.60           | 0.82            | 1.02            | -0.05           | 0.97            |
|                      | AVQZ      | 0.26           | 0.16           | 0.24            | 0.34            | 0.00            | 0.31            |
|                      | AVSZ      | 0.15           | 0.08           | 0.14            | 0.19            | -0.01           | 0.17            |
|                      | AV\{T,Q\}Z | 0.12           | 0.13           | 0.14            | 0.10            | 0.04            | 0.13            |
|                      | AV\{Q,5\}Z | 0.03           | 0.01           | 0.04            | 0.04            | -0.01           | 0.05            |
| LNO-CCSD(T) vTight   | AVTZ      | 0.77           | 0.51           | 0.71            | 0.97            | 0.00            | 0.90            |
|                      | AVQZ      | 0.22           | 0.11           | 0.16            | 0.32            | 0.04            | 0.27            |
|                      | AVSZ      | 0.10           | 0.04           | 0.07            | 0.17            | 0.03            | 0.13            |
|                      | AV\{T,Q\}Z | 0.15           | 0.15           | 0.20            | 0.11            | 0.06            | 0.16            |
|                      | AV\{Q,5\}Z | 0.03           | 0.05           | 0.04            | 0.02            | 0.03            | 0.04            |
| LNO-CCSD(T) vvTight  | AVTZ      | 0.77           | 0.50           | 0.71            | 0.96            | 0.00            | 0.89            |
|                      | AVQZ      | 0.06           | 0.04           | 0.04            | 0.09            | 0.02            | 0.07            |
|                      | AVSZ      | 0.10           | 0.12           | 0.13            | 0.05            | 0.09            | 0.11            |
|                      | AV\{T,Q\}Z | 0.09           | 0.11           | 0.16            | —               | —               | —               |
|                      | AV\{Q,5\}Z | 0.15           | 0.18           | 0.21            | 0.09            | 0.14            | 0.17            |
| PNO-LCCSD(T) Default | AVTZ      | 0.06           | 0.04           | 0.04            | 0.09            | 0.02            | 0.07            |
|                      | AVQZ      | 0.10           | 0.12           | 0.13            | 0.05            | 0.09            | 0.11            |
|                      | AVSZ      | —              | 0.10           | 0.16            | —               | —               | —               |
|                      | AV\{T,Q\}Z | 0.15           | 0.18           | 0.21            | 0.09            | 0.14            | 0.17            |
|                      | AV\{Q,5\}Z | 0.03           | 0.08           | 0.18            | —               | —               | —               |
| PNO-LCCSD(T) Tight   | AVTZ      | 0.12           | 0.07           | 0.12            | 0.14            | -0.02           | 0.13            |
|                      | AVQZ      | 0.09           | 0.11           | 0.11            | 0.07            | 0.09            | 0.10            |
|                      | AVSZ      | —              | 0.10           | —               | —               | —               | —               |
|                      | AV\{T,Q\}Z | 0.18           | 0.23           | 0.26            | 0.08            | 0.16            | 0.20            |
|                      | AV\{Q,5\}Z | 0.20           | 0.23           | 0.29            | —               | —               | —               |
| DLPNO-CCSD(T) \(_0\) NormalPNO | AVTZ      | 0.77           | 0.68           | 0.90            | 0.72            | -0.22           | 0.84            |
|                      | AVQZ      | 0.33           | 0.32           | 0.41            | 0.26            | -0.14           | 0.36            |
|                      | AVSZ      | 0.24           | 0.28           | 0.35            | 0.14            | -0.16           | 0.28            |
|                      | AV\{T,Q\} | 0.09           | 0.09           | 0.09            | 0.10            | -0.09           | 0.10            |
|                      | AV\{Q,5\} | 0.20           | 0.23           | 0.29            | 0.11            | -0.19           | 0.23            |
| DLPNO-CCSD(T) \(_0\) TightPNO T\(_{CutPNO}=10^{-6}\) | AVTZ      | 0.56           | 0.30           | 0.45            | 0.78            | 0.07            | 0.67            |
|                      | AVQZ      | 0.13           | 0.10           | 0.11            | 0.17            | -0.01           | 0.15            |
|                      | AVSZ      | —              | 0.16           | —               | —               | —               | —               |
|                      | AV\{T,Q\} | 0.17           | 0.05           | 0.12            | 0.27            | -0.06           | 0.22            |
|                      | AV\{Q,5\} | —              | 0.42           | —               | —               | —               | —               |
| DLPNO-CCSD(T) \(_0\) TightPNO T\(_{CutPNO}=10^{-7}\) | AVTZ      | 0.67           | 0.38           | 0.57            | 0.91            | 0.06            | 0.79            |
|                      | AVQZ      | 0.18           | 0.04           | 0.08            | 0.35            | 0.11            | 0.26            |
|                      | AVSZ      | —              | 0.05           | —               | —               | —               | —               |
|                      | AV\{T,Q\} | 0.18           | 0.23           | 0.28            | 0.06            | 0.14            | 0.22            |
|                      | AV\{Q,5\} | —              | 0.11           | —               | —               | —               | —               |
| DLPNO-CCSD(T) \(_0\) TightPNO | AVTZ      | 0.72           | 0.42           | 0.62            | 0.98            | 0.05            | 0.86            |
| T$\text{CutPNO}=10^{-6,7}$ | AVQZ | 0.23 | 0.06 | 0.10 | 0.44 | 0.17 | 0.33 |
|---------------------------|------|------|------|------|------|------|------|
| or CPS{6,7}[a]           | AV5Z | —    | 0.02 | —    | —    | —    | —    |
|                           | AV{T,Q} | 0.26 | 0.33 | 0.37 | 0.14 | 0.25 | 0.29 |
| VeryTightPNO              | AV{T,Q}| —    | 0.05 | —    | —    | —    | —    |
|                           | AVTZ | 0.61 | 0.36 | 0.53 | 0.81 | 0.05 | 0.71 |
|                           | AVQZ | —    | 0.01 | —    | —    | —    | —    |
|                           | AV{T,Q} | —    | 0.25 | —    | —    | —    | —    |
| DLPNO-CCSD($T_1$)         | NormalPNO | AVTZ | 0.79 | 0.70 | 0.93 | 0.72 | -0.23 | 0.86 |
|                           | AVQZ | 0.34 | 0.35 | 0.44 | 0.26 | -0.16 | 0.38 |
|                           | AV5Z | 0.26 | 0.30 | 0.38 | 0.14 | -0.18 | 0.30 |
|                           | AV{T,Q}Z | 0.11 | 0.11 | 0.12 | 0.11 | -0.10 | 0.12 |
|                           | AV{Q,5}Z | 0.22 | 0.25 | 0.32 | 0.12 | -0.20 | 0.25 |
| TightPNO                  | AVTZ | 0.58 | 0.32 | 0.49 | 0.81 | 0.06 | 0.69 |
| T$\text{CutPNO}=10^{-6}$  | AVQZ | 0.15 | 0.05 | 0.07 | 0.27 | 0.12 | 0.20 |
|                           | AV5Z | —    | 0.13 | —    | —    | —    | —    |
|                           | AV{T,Q}Z | 0.24 | 0.29 | 0.34 | 0.12 | 0.16 | 0.27 |
|                           | AV{Q,5}Z | —    | 0.22 | —    | —    | —    | —    |
| TightPNO                  | AVTZ | 0.70 | 0.41 | 0.60 | 0.94 | 0.05 | 0.82 |
| T$\text{CutPNO}=10^{-7}$  | AVQZ | 0.20 | 0.05 | 0.09 | 0.37 | 0.10 | 0.28 |
|                           | AV5Z | —    | 0.03 | —    | —    | —    | —    |
|                           | AV{T,Q}Z | 0.16 | 0.20 | 0.25 | 0.06 | 0.13 | 0.19 |
|                           | AV{Q,5}Z | —    | 0.08 | —    | —    | —    | —    |
| TightPNO                  | AVTZ | 0.76 | 0.45 | 0.66 | 1.01 | 0.05 | 0.89 |
| T$\text{CutPNO}=10^{-6,7}$| AVQZ | 0.25 | 0.08 | 0.14 | 0.43 | 0.09 | 0.33 |
| or CPS{6,7}[a]           | AV5Z | —    | 0.04 | —    | —    | —    | —    |
|                           | AV{T,Q}Z | 0.14 | 0.16 | 0.20 | 0.07 | 0.12 | 0.16 |
|                           | AV{Q,5}Z | —    | 0.02 | —    | —    | —    | —    |
| VeryTightPNO              | AVTZ | 0.64 | 0.39 | 0.56 | 0.84 | 0.04 | 0.75 |
|                           | AVQZ | —    | 0.02 | —    | —    | —    | —    |
|                           | AV{T,Q}Z | —    | 0.23 | —    | —    | —    | —    |

[a] The expression CPS{X,Y} refers to the extrapolation of $T_{\text{CutPNO}}$ to the complete PNO space limit using $T_{\text{CutPNO}}=10^{-X}$ and $10^{-Y}$, where $Y=X+1$
**Table S8**: Performance of standard and composite PNO-LCCSD(T) methods with respect to the revised reference conformer energies of longer n-alkanes. The default "REXT" setting for the "Tight" and "Default" domains (7 and 5 bohr, respectively) were used throughout. Heatmapping is from red (worst) via yellow to green (best).

| Threshold | Basis set                | $c_1$ | MAD (kcal/mol) |          | MSD (kcal/mol) | RMSD (kcal/mol) |
|-----------|--------------------------|-------|----------------|----------|----------------|-----------------|
|           |                          |       | ACONFL        | ACONF12  | ACONF16        | ACONF20         |
| Default   | AVTZ                     | 0.05  | 0.04           | 0.06     | 0.05           | 0.02            | 0.06            |
|           | AVQZ                     | 0.10  | 0.11           | 0.15     | 0.05           | 0.07            | 0.12            |
|           | AV5Z                     | 0.16  | 0.17           | 0.22     | 0.10           | 0.11            | 0.18            |
|           | AV[T,Q]Z                 | 0.16  | 0.17           | 0.22     | 0.10           | 0.11            | 0.18            |
|           | AV{Q,5}Z                 | 0.09  |                |          |                |                 |
| Tight     | AVTZ                     | 0.42  | 0.37           | 0.46     | 0.41           | -0.10           | 0.46            |
|           | AVQZ                     | 0.05  | 0.02           | 0.02     | 0.09           | 0.03            | 0.07            |
|           | AV5Z                     | 0.05  |                |          |                |                 |
|           | AV{T,Q}Z                 | 0.21  | 0.22           | 0.29     | 0.15           | 0.12            | 0.23            |
|           | AV{Q,5}Z                 | 0.11  |                |          |                |                 |
| Composite methods\[^a\] | Default {T,Q} + $c_1$[Tight – Default]/T | 0.39 | 0.06 | 0.01 | 0.03 | 0.12 | 0.06 | 0.08 |
| Composite methods\[^b\] | Tight {T,Q} + $c_1$[Tight – Default]/T | 0.30 | 0.09 | 0.10 | 0.13 | 0.06 | 0.08 | 0.11 |
|             | Tight {T,Q} + $c_1$[Tight-Default]/Q | 0.66 | 0.12 | 0.14 | 0.18 | 0.07 | 0.09 | 0.14 |
| Composite methods\[^b\] | Default {T,Q} + $c_1$[Tight – Default]/T | 0.40 | 0.06 | 0.01 | 0.03 | 0.12 | 0.06 | 0.09 |
| Composite methods\[^b\] | Tight {T,Q} + $c_1$[Tight – Default]/T | 0.53 | 0.06 | 0.01 | 0.03 | 0.11 | 0.05 | 0.07 |
|             | Tight {T,Q} + $c_1$[Tight-Default]/Q | 1.53 | 0.05 | 0.03 | 0.04 | 0.08 | 0.05 | 0.06 |

\[^a\] Coefficients are taken from the "raw" category of Table 4 in Ref. 2

\[^b\] Coefficients are reoptimized relative to the revised ACONFL reference data.
Table S9: Performance of explicitly correlated PNO-LCCSD(T)-F12b with respect to the revised reference conformer energies of longer n-alkanes. The default “REXT” setting for the “Tight” and “Default” domains (7 and 5 a.u., respectively) were used throughout. Heatmapping is from red (worst) via yellow to green (best).

| Methods          | Threshold | Basis set | MAD (kcal/mol) | MSD (kcal/mol) | RMSD (kcal/mol) |
|------------------|-----------|-----------|----------------|---------------|-----------------|
|                  |           |           | ACONFL | ACONF12 | ACONF16 | ACONF20 |         |         |
| PNO-LCCSD(T)-F12b| Default   | VDZ-F12   | 0.17   | 0.08    | 0.12    | 0.26    | -0.05 | 0.20    |
|                  |           | VTZ-F12   | 0.16   | 0.14    | 0.19    | 0.15    | 0.04  | 0.18    |
|                  |           | VQZ-F12   |        | 0.10    |         |         |       |         |
|                  | Tight     | VDZ-F12   | 0.16   | 0.13    | 0.16    | 0.17    | 0.01  | 0.17    |
|                  |           | VTZ-F12   | 0.13   | 0.12    | 0.16    | 0.12    | 0.04  | 0.14    |
| PNO-LCCSD(Ts)-F12b[a] | Default | VDZ-F12   | 0.10   | 0.02    | 0.04    | 0.18    | -0.06 | 0.13    |
|                  |           | VTZ-F12   | 0.13   | 0.12    | 0.15    | 0.12    | 0.04  | 0.14    |
|                  |           | VQZ-F12   |        | 0.09    |         |         |       |         |
|                  | Tight     | VDZ-F12   | 0.08   | 0.06    | 0.07    | 0.09    | 0.00  | 0.08    |
|                  |           | VTZ-F12   | 0.10   | 0.09    | 0.12    | 0.08    | 0.03  | 0.10    |

[a]Following Ref.², the (T) terms of PNO-LCCSD(T)-F12b and DLPNO-CCSD(Ts)-F12 were scaled by 1.1413, 1.0527, and 1.0232 for VDZ-F12, VTZ-F12, and VQZ-F12, respectively.
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