**Table 9.** Geometrical parameters for the optimized $[(CO)_2Re(C_5H_4)C{\equiv}C(C_5H_4)Re[(CO)_2]$(alkane) complexes, calculated at the BP86/ 6-31G*, LANL2DZ level of theory

| **DFT(BP86)** | *Interacting Pair of Atoms* | *M-H Distance* | *M-C distance* | *M-H-C angle* | *C-H bound distance* | *Average C-H free distance* |
|---|---|---|---|---|---|---|
| Methane | $Re_1$-C | 1.946 | 2.634 | 113.303 | 1.164 | 1.100 |
| | $Re_2$-C | | 4.119 | | | |
| Ethane | $Re_1$-C1 | 1.973 | 2.745 | 120.500 | 1.154 | 1.101 |
| | $Re_2$-C2 | 1.975 | 2.747 | 120.412 | 1.156 | 1.100 |
| Propane | $Re_1$-C1 | 1.952 | 2.716 | 119.456 | 1.159 | 1.102 |
| | $Re_2$-C3 | 1.995 | 2.829 | 125.554 | 1.156 | 1.101 |
| Butane | $Re_1$-C1 | 1.951 | 2.718 | 119.872 | 1.155 | 1.103 |
| | $Re_2$-C4 | 1.958 | 2.731 | 120.557 | 1.153 | 1.102 |
| Pentane | $Re_1$-C1 | 1.965 | 2.792 | 124.766 | 1.158 | 1.100 |
| | $Re_2$-C5 | 1.985 | 2.870 | 130.260 | 1.154 | 1.099 |
| Cyclopropane | $Re_1$-C1 | 1.979 | 2.671 | 114.669 | 1.148 | 1.090 |
| | $Re_2$-C2 | 1.987 | 2.710 | 117.514 | 1.141 | 1.090 |
| Cyclobutane | $Re_1$-C1 | 1.88 | 2.66 | 119.44 | 1.17 | 1.101 |
| Cyclopentane | $Re_1$-C1 | 1.939 | 2.838 | 130.372 | 1.167 | 1.098 |
| | $Re_2$-C2 | 1.972 | 2.754 | 120.861 | 1.161 | 1.100 |
| Cyclohexane | $Re_1$-C1 | 2.01 | 3.01 | 141.605 | 1.162 | 1.102 |
| | $Re_2$-C2 | 2.14 | 2.91 | 121.013 | 1.146 | 1.104 |

"M-H distance" and "M-C distance" are the distances between the designated Re atom ("M" = $Re_1$ or $Re_2$) and the H and C atoms, respectively, of the C-H σ-bond that interacts most strongly with that particular Re atom (i.e. the C-H σ-bond that lies in closest proximity to that Re atom). The designations "C1", "C2", etc. indicate the position along the alkane chain / ring of the $CH_3$ / $CH_2$ group that is interacting with the designated Re atom. "M-H-C angle" is the angle between the Re atom and the aforementioned C-H bond. "C-H bound distance" is the length of the aforementioned C-H bond. "Average C-H free distance" is the average length of the remaining C-H bonds that are located on the same $CH_3$ (linear alkanes)/ $CH_2$ (cyclic alkanes) group as the interacting bond (in the case of cyclic alkanes, "Average C-H free distance" is simply one bond length, not an average of two lengths).