Table 5. Geometrical parameters for the optimized [$CpRe(CO)_2$](alkane) complexes, calculated at the BP86/ 6-31G*, LANL2DZ level of theory

DFT, BP86	**M-H distance**	**M-C distance**	**M-H-C angle**	**C-H bound distance**	**Average C-H free distance**
Methane	1.97	2.67	114.68	1.16	1.10
Ethane	1.95	2.71	118.91	1.16	1.10
Propane	1.96	2.70	118.05	1.16	1.11
Butane	1.95	2.70	118.19	1.16	1.10
Pentane	1.93	2.70	119.07	1.17	1.11
Hexane	1.96	2.69	116.63	1.16	1.10
Heptane	1.95	2.69	117.30	1.16	1.11
Cyclopropane	1.92	2.58	111.53	1.16	1.09
Cyclobutane	1.91	2.70	120.85	1.17	1.10
Cyclopentane	1.91	2.72	122.40	1.17	1.10
Cyclohexane	1.93	2.71	119.91	1.17	1.10

"M-H distance" and "M-C distance" are the distances between the Re atom ("M") and the H and C atoms, respectively, of the C-H σ-bond that interacts most strongly with the Re atom (i.e. the C-H σ-bond that lies in closest proximity to the 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).