Table 8. Geometrical parameters for the optimized $[(CO)_2Re(C_5H_4)C{\equiv}C(C_5H_4)Re[(CO)_2]$(alkane) complexes, calculated at the B3LYP/ 6-31G*, LANL2DZ level of theory

DFT(B3LYP)	*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	1.979	2.740	120.688	1.138	1.091
	Re_2-C		4.751			
Ethane	Re_1-C1	2.031	2.813	122.901	1.133	1.092
	Re_2-C2	2.016	2.818	124.552	1.134	1.091
Propane	Re_1-C1	2.039	2.899	129.745	1.135	1.092
	Re_2-C3	1.988	2.786	123.795	1.137	1.092
Butane	Re_1-C1	1.988	2.771	122.737	1.135	1.093
	Re_2-C4	1.993	2.780	123.256	1.134	1.093
Pentane	Re_1-C1	1.993	2.850	129.057	1.138	1.091
	Re_2-C5	2.024	2.910	132.085	1.136	1.091
Cyclopropane	Re_1-C1	2.023	2.818	124.807	1.122	1.081
	Re_2-C2	2.020	2.834	126.632	1.120	1.082
Cyclobutane	Re_1-C1	1.94	2.75	123.90	1.15	1.090
Cyclopentane	Re_1-C1	2.108	3.035	138.863	1.111	1.079
	Re_2-C2	2.107	3.003	135.668	1.110	1.078

"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).