Table 10. Table 10. Geometrical parameters for the optimized $[(CO)_2Re(C_5H_4)C{\equiv}C(C_5H_4)Re[(CO)_2]$(alkane) complexes, calculated at the SOS-MP2/ 6-31G*, LANL2DZ, RIMP2-VDZ (auxiliary basis set) level of theory

SOS-MP2	*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	2.032	2.738	116.727	1.137	1.087
	Re_2-C	2.026	2.728	116.278	1.137	1.087
Ethane	Re_1-C1	1.985	2.736	120.044	1.136	1.092
	Re_2-C2	1.988	2.722	118.743	1.135	1.092
Butane	Re_1-C1	1.991	2.692	116.293	1.135	1.094
	Re_2-C4	1.994	2.690	115.797	1.135	1.094
Pentane	Re_1-C1	1.941	2.741	123.435	1.142	1.092
	Re_2-C5	1.950	2.809	129.249	1.135	1.092

"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).