Table 11. Geometrical parameters for the optimized $[(CO)_2Re(C_5H_4)C{\equiv}C(C_5H_4)Re[(CO)_2]$(alkane) complexes, calculated at the RIMP2/ 6-31G*, LANL2DZ, RIMP2-VDZ (auxiliary basis set) level of theory

RIMP2	*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	1.98	2.62	111.28	1.15	1.09
	Re_2-C	1.99	2.64	111.93	1.15	1.09
Ethane	Re_1-C1	1.92	2.58	111.98	1.15	1.09
	Re_2-C2	1.92	2.58	111.57	1.15	1.09
Propane	Re_1-C1	1.91	2.70	121.88	1.15	1.09
	Re_2-C3	1.91	2.57	111.49	1.15	1.10
Butane	Re_1-C1	1.95	2.61	112.84	1.15	1.09
	Re_2-C4	1.95	2.61	112.42	1.15	1.09
Pentane	Re_1-C1	1.91	2.74	126.30	1.14	1.09
	Re_2-C5	1.90	2.66	118.82	1.15	1.09
Cyclopropane	Re_1-C1	1.94	2.50	105.18	1.14	1.08
	Re_2-C2	1.93	2.52	106.99	1.14	1.08
Cyclopentane	Re_1-C1	1.89	2.66	119.96	1.16	1.09
	Re_2-C2	1.89	2.62	116.19	1.16	1.09
Propane	Re_1-C1	1.91	2.70	121.88	1.15	1.09
	Re_2-C3	1.91	2.57	111.49	1.15	1.10
Butane	Re_1-C1	1.95	2.61	112.84	1.15	1.09
	Re_2-C4	1.95	2.61	112.42	1.15	1.09
Pentane	Re_1-C1	1.91	2.74	126.30	1.14	1.09
	Re_2-C5	1.90	2.66	118.82	1.15	1.09

Cyclopropane	Re_1-C1	1.94	2.50	105.18	1.14	1.08
	Re_2-C2	1.93	2.52	106.99	1.14	1.08
Cyclopentane	Re_1-C1	1.89	2.66	119.96	1.16	1.09
	Re_2-C2	1.89	2.62	116.19	1.16	1.09

"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).