Table 3. [CpRe(CO)2](heptane)/(pentane) binding energies (kcal/mol) for various binding modes

Pentane	***C1***	***C2***	***C3***
Uncorrected Binding Energy	9.595	8.596	8.610
BSSE	1.755	2.124	2.019
	7.840	6.472	6.591

Heptane	***C1***	***C2***	***C3***	***C4***
Uncorrected Binding Energy	9.678	8.826	8.707	8.695
BSSE	1.756	2.480	2.443	2.411
Corrected BE	7.922	6.345	6.265	6.284

Calculations were performed at the B3LYP/6-31G*, LANL2DZ level. C1 indicates a terminal carbon; C4 is the central carbon for heptane, and C3 the central carbon for pentane.