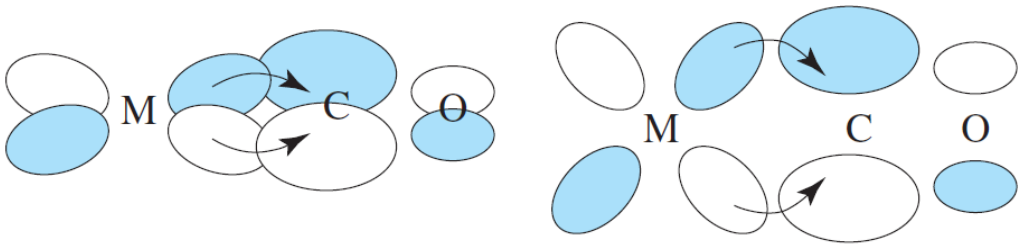

Table 5. M−CO and C−O Bond Lengths (Å) of $M(CO)_5$

	$Fe(CO)_5$				$Ru(CO)_5$				$Os(CO)_5$			
method	$M-C_{ax}$	$M-C_{eq}$	$C-O_{ax}$	$C-O_{eq}$	$M-C_{ax}$	$M-C_{eq}$	$C-O_{ax}$	$C-O_{eq}$	$M-C_{ax}$	$M-C_{eq}$	$C-O_{ax}$	$C-O_{eq}$
LDA	1.769	1.789	1.145	1.149	1.934	1.931	1.142	1.147	2.003	1.988	1.140	1.147
NL-SCF	1.819	1.816	1.153	1.157	1.983	1.980	1.149	1.154	2.061	2.050	1.147	1.153
NL-SCF+QR	1.817	1.813	1.153	1.156	1.968	1.960	1.150	1.157	2.000	1.975	*1.147*	*1.156*
MRCI[a]	1.798	1.835										
MCPF[b]	1.878	1.847	1.168	1.177								
exp[c]	1.807	1.827	1.152	1.152	1.950[d]	1.969[d]	1.143	1.143	1.990[e]	1.943[e]	1.142	1.142

[a] Reference 41. [b] Reference 39. [c] $Fe(CO)_5$ from ref 41, $Ru(CO)_5$ from ref 42, $Os(CO)_5$ from ref 43. [d] Estimated errors are 0.01 Å for Ru−CO bonds. [e] Estimated errors are 0.02 Å for Os−CO bonds.