Binuclear Manganese and Rhenium Carbonyls $M_2(CO)_n$ (n = 10, 9, 8, 7): Comparison of First Row and Third Row Transition Metal Carbonyl Structures

Bing Xu,[a] Qian-Shu Li,[*a,b] Yaoming Xie,[c] R. Bruce King,[*c] and Henry F. Schaefer III[c]

[a]*Institute of Chemical Physics, Beijing Institute of Technology, Beijing 100081, China*
[b]*Center for Computational Quantum Chemistry, South China Normal University, Guangzhou, 510631 China*
[c]*Department of Chemistry and Center for Computational Chemistry University of Georgia, Athens, Georgia 30602, USA*
e-mails: rbking@chem.uga.edu and qsli@scnu.edu.cn

Supporting Information

Figures S1 to S7 and Tables S1 to S13: Optimized structures, total energies, relative energies, imaginary vibrational frequencies, and ν(CO) frequencies for $Re_2(CO)_{10}$ (3 isomers), $Re_2(CO)_9$ (8 isomers), $Re_2(CO)_8$ (17 isomers) and $Re_2(CO)_7$ (10 isomers)

Complete Gaussian 03 reference (Reference 30)

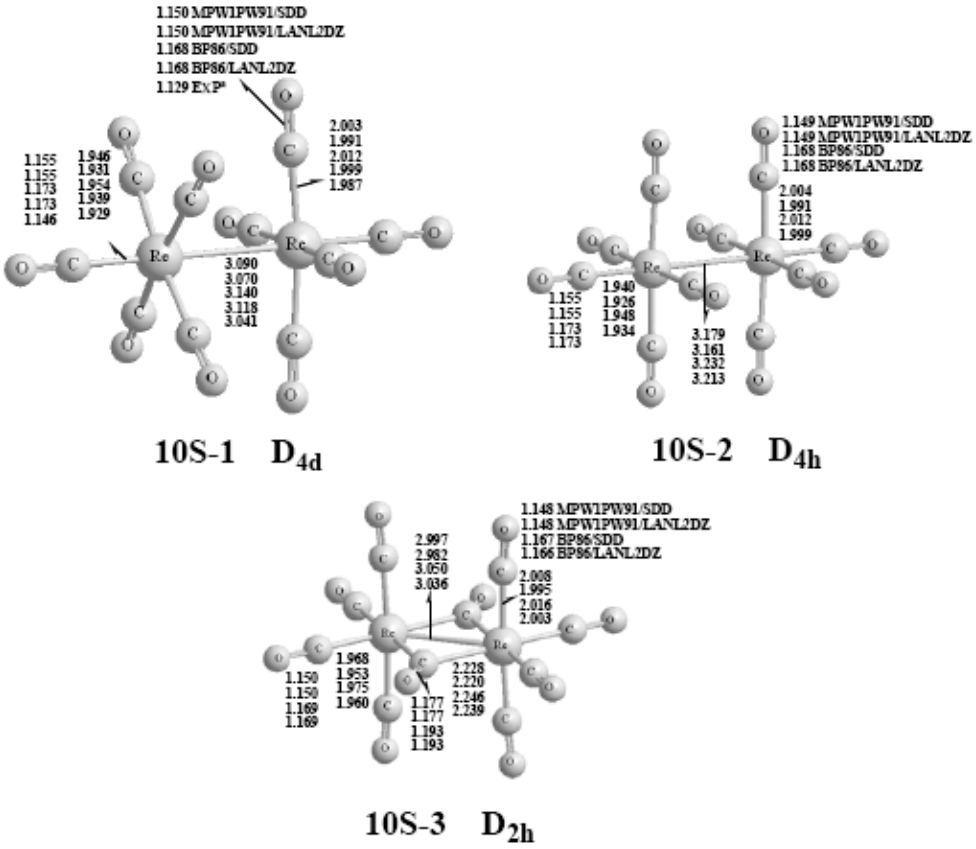

Figure S1. The optimized structures of $Re_2(CO)_{10}$.

Table S1. The total energies (E, in Hartree) and relative energies (ΔE, in kcal/mol) of $Re_2(CO)_{10}$. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure are also listed.

		10S-1 (D_{4d})	**10S-2** (D_{4h})	**10S-3** (D_{2h})
MPW1PW91/ SDD	E	-1290.21336	-1290.20633	-1290.16672
	ΔE	0	4.4	29.3
	Nimag	0	1(18i)	1(150i)
	Re-Re	3.090	3.179	2.997
BP86/ SDD	E	-1290.76883	-1290.76301	-1290.72988
	ΔE	0	3.7	24.4
	Nimag	0	1(14i)	1(134i)
	Re-Re	3.140	3.232	3.050
MPW1PW91/ LANL2DZ	E	-1291.77740	-1291.77025	-1291.72953
	ΔE	0	4.5	30
	Nimag	0	1(20i)	1(158i)
	Re-Re	3.070	3.161	2.982
BP86/ LANL2DZ	E	-1292.27936	-1292.27328	-1292.23903
	ΔE	0	3.8	25.3
	Nimag	0	1(16i)	1(144i)
	Re-Re	3.118	3.213	3.036

Table S2. The active infrared ν(CO) vibrational frequencies (cm^{-1}) predicted for $Re_2(CO)_{10}$ (infrared intensities in parentheses are in km/mol, bridging ν(CO) frequencies are in **bold**).

	MPW1PW91/ SDD	MPW1PW91/ LANL2DZ	BP86/ SDD	BP86/ LANL2DZ
10S-1(D_{4d})	2089(1630), 2124(2950), 2172(1078)	2095(1575), 2127(2925), 2176(1092)	1974(1368), 2002(2484), 2052(934)	1981(1305), 2006(2458), 2056(955)
10S-2(D_{4h})	2089(1475), 2128(2902), 2173(1327)	2095(1412), 2131(2873), 2177(1351)	1975(1241), 2006(2434), 2053(1128)	1982(1170), 2009(2403), 2057(1158)
10S-3(D_{2h})	**1883(1099),** 2123(1067), 2123(2046), 2130(3008), 2175(1736)	**1889(1115),** 2127(1044), 2129(2007), 2134(2965), 2179(1735)	**1800(839),** 1999(762), 2001(1721), 2005(2533), 2048(1721)	**1805(854),** 2004(734), 2007(1683), 2009(2492), 2053(1716)

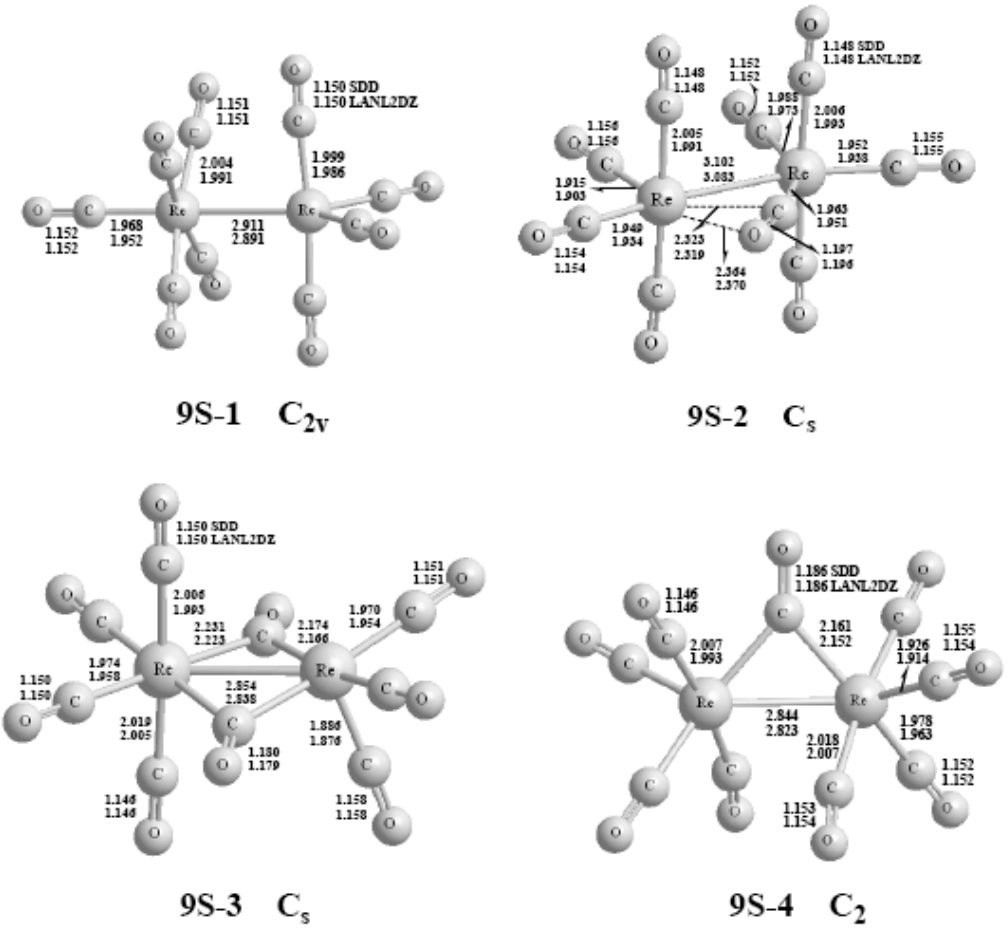

Figure S2. The optimized singlet structures of $Re_2(CO)_9$ by MPW1PW91 method.

Table S3. The total energies (E, in Hartree) and relative energies (ΔE, in kcal/mol) of singlet structures of $Re_2(CO)_9$. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure are also listed.

		9S-1 (C_{2v})	**9S-2** (C_s)	**9S-3** (C_s)	**9S-4** (C_2)
MPW1PW91/ SDD	E	-1176.84455	-1176.84420	-1176.80326	-1176.79807
	ΔE	0	0.2	25.9	29.2
	Nimag	0	0	1(117i)	1(100i)
	Re-Re	2.911	3.102	2.854	2.844
MPW1PW91/ LANL2DZ	E	-1178.40789	-1178.40675	-1178.36509	-1178.35932
	ΔE	0	0.7	26.9	30.5
	Nimag	0	0	1(125i)	2(115i,9i)
	Re-Re	2.891	3.083	2.838	2.823
BP86/SDD	E	-1177.36824	-1177.36957	-1177.33418	-1177.33060
	ΔE	0	0.8	21.4	23.6
	Nimag	0	0	1(136i)	2(89i,12i)
	Re-Re	2.939	3.144	2.881	2.882

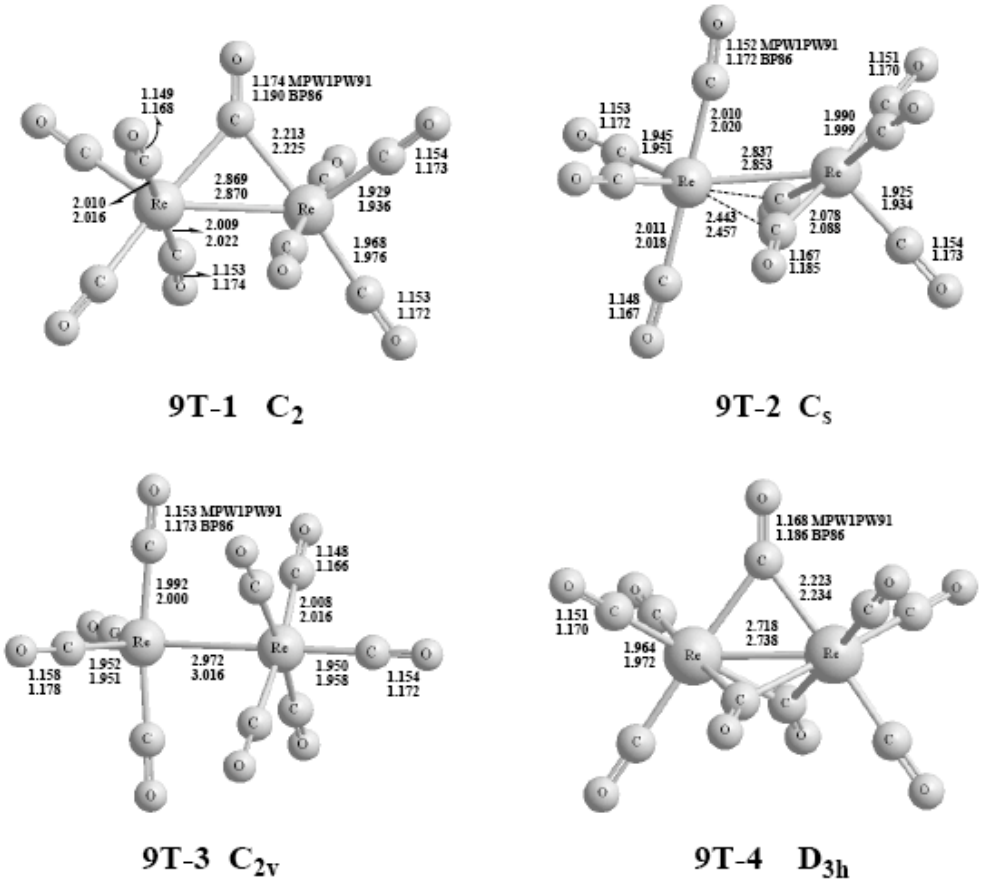

Figure S3. The four optimized triplet structures of $Re_2(CO)_9$ by SDD basis sets. .

Table S4. The total energies (E, in Hartree) and relative energies (ΔE, in kcal/mol) of triplet structures of $Re_2(CO)_9$. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure is also listed.

		9T-1 (C_2)	**9T-2** (C_s)	**9T-3** (C_{2v})	**9T-4** (D_{3h})
MPW1PW91/ SDD	E	-1176.80134	-1176.79893	-1176.79892	-1176.79307
	ΔE	27.1	28.6	28.6	32.3
	Nimag	0	1(99i)	0	2(92i,92i)
	Re-Re	2.869	2.837	2.972	2.718
BP86/SDD	E	-1177.32944	-1177.32839	-1177.32610	-1177.32308
	ΔE	24.3	25.0	26.4	28.3
	Nimag	0	1(59i)	0	2(116i,116i)
	Re-Re	2.870	2.853	3.016	2.738

Table S5. The infrared ν(CO) vibrational frequencies (cm^{-1}) predicted for $Re_2(CO)_9$ (infrared intensities in parentheses are in km/mol, bridging ν(CO) frequencies are in **bold**).

	MPW1PW91/SDD	BP86/SDD	MPW1PW91/LANL2DZ
9S-1 (C_{2v})	2069(551), 2080(22), 2093(1004), 2105(2186), 2108(305), 2119(2963), 2126(0), 2163(1099), 2215(22)	1954(437), 1960(87), 1974(728), 1987(1847), 1988(334), 1997(2393), 2006(0), 2039(962), 2087(37)	2074(517), 2083(30), 2098(973), 2109(2194), 2113(298), 2122(2928), 2130(0), 2167(1109), 2219(21)
9S-2 (C_s)	**1836(548),** 2079(520), 2094(39), 2095(1365), 2106(785), 2124(541), 2128(3008), 2175(1007), 2217(52)	**1728(458),** 1966(485), 1972(84), 1979(1015), 1985(596), 2002(519), 2004(2480), 2051(923), 2088(45)	**1844(544),** 2086(508), 2097(30), 2101(1320), 2111(772), 2129(529), 2131(2980), 2179(1022), 2221(54)
9S-3 (C_s)	**1869(1005), 1920(30),** 2077(499), 2113(1650), 2114(393), 2127(1615), 2137(1287), 2155(1876), 2210(134)	**1789(771), 1820(48),** 1965(381), 1986(433), 1988(1404), 2002(1245), 2010(972), 2028(1780), 2078(151)	**1874(1020), 1924(29),** 2084(460), 2117(1693), 2119(433), 2132(1531), 2141(1225), 2159(1875), 2214(131)
9S-4 (C_2)	**1862(561),** 2072(42), 2083(46), 2095(902), 2101(2327), 2122(1194), 2131(1530), 2168(1973), 2210(10)	**1778(433),** 1953(65), 1962(70), 1976(692), 1980(1869), 1995(911), 2001(1296), 2039(1827), 2078(6)	**1867(569),** 2076(65), 2087(110), 2101(904), 2105(2229), 2126(1201), 2134(1439), 2170(2005), 2214(9)
9T-1 (C_2)	**1945(401),** 2074(40), 2084(304), 2093(903), 2095(2146), 2112(170), 2112(2190), 2150(2263), 2201(5)	**1838(360),** 1946(150), 1953(658), 1974(269), 1978(1669), 1987(109), 1988(1664), 2022(2245), 2068(2)	
9T-2 (C_s)	**1981(741), 1983(187),** 2086(143), 2094(796), 2101(1618), 2106(1261), 2116(1223), 2146(2557), 2199(19)	**1869(633), 1872(152),** 1961(342), 1976(562), 1982(1041), 1985(1095), 1990(985), 2022(2338), 2067(9)	
9T-3 (C_{2v})	2053(1261), 2057(852), 2063(618), 2099(599), 2119(1864), 2124(2394), 2137(964), 2143(0), 2219(159)	1935(690), 1936(890), 1943(545), 1982(575), 1997(1543), 2000(1919), 2013(747), 2019(0), 2090(155)	
9T-4 (D_{3h})	**1958(758), 1958(758), 2006(0),** 2105(0), 2105(0), 2112(1974), 2112(1974), 2150(2770), 2193(0)	**1852(629), 1852(629), 1882(0),** 1983(0), 1983(0), 1990(1610), 1990(1610), 2024(2482), 2063(0)	**1962(763), 1962(763), 2009(0),** 2111(0), 2111(0), 2118(1940), 2118(1940), 2155(2728), 2198(0)

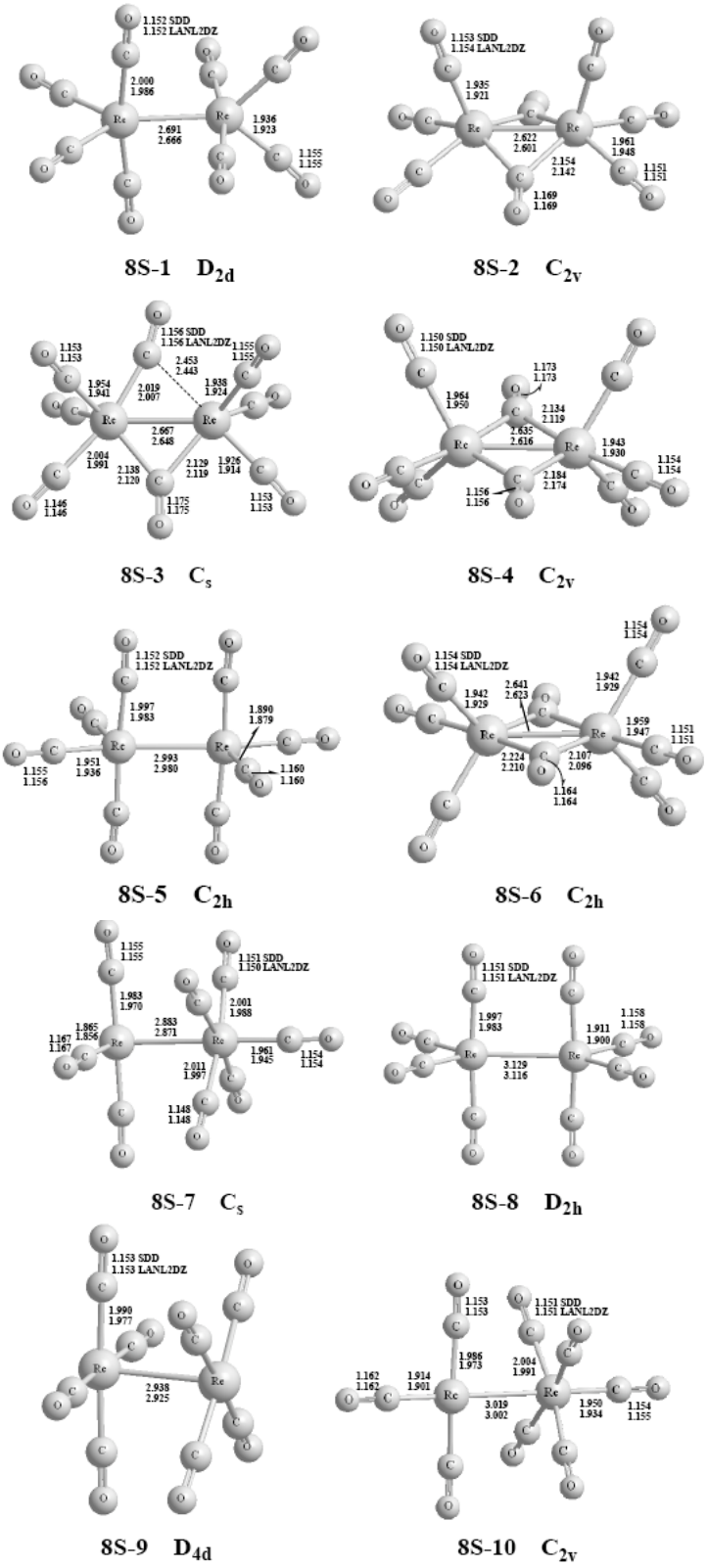

Figure S4. The optimized ten singlet structures of $Re_2(CO)_8$ by the MPW1PW91 method.

Table S6. The total energies (E, in Hartree) and relative energies (ΔE, in kcal/mol) of singlet structures of $Re_2(CO)_8$. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure are also listed.

	8S-1 (D_{2d})	**8S-2** (C_{2v})	**8S-3** (C_s)	**8S-4** (C_{2v})	**8S-5** (C_{2h})
MPW1PW91/SDD					
E	-1063.48100	-1063.46028	-1063.45735	-1063.45483	-1063.45249
ΔE	0	13	14.8	16.4	17.9
Nimag	0	0	1(20i)	2(232i,38i)	1(37i)
Re-Re	2.691	2.622	2.667	2.635	2.993
MPW1PW91/LANL2DZ					
E	-1065.04430	-1065.02017	-1065.01787	-1065.01514	-1065.01425
ΔE	0	15.1	16.6	18.3	18.9
Nimag	0	0	1(17i)	2(231i,36i)	1(38i)
Re-Re	2.666	2.601	2.648	2.616	2.980
BP86/SDD					
E	-1063.97512	-1063.96332	-1063.95909	-1063.95776	-1063.94449
ΔE	0	7.4	10.1	10.9	19.2
Nimag	0	0	1(19*i*)	2(180*i*,36*i*)	2(37*i*,5*i*)
Re-Re	2.699	2.660	2.702	2.680	3.010

Table S7. The total energies (E, in Hartree) and relative energies (ΔE, in kcal/mol) of singlet $Re_2(CO)_8$ structures. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure are also listed.

	8S-6 (C_{2h})	**8S-7** (C_s)	**8S-8** (D_{2h})	**8S-9** (D_{4d})	**8S-10** (C_{2v})
MPW1PW91/SDD					
E	-1063.45026	-1063.44485	-1063.44438	-1063.4149	-1063.40935
ΔE	19.3	22.7	23.0	41.5	45.0
Nimag	3(72i,19i,16i)	0	3(56i,40i,18i)	0	1(120i)
Re-Re	2.641	2.883	3.129	2.938	3.019
MPW1PW91/LANL2DZ					
E	-1065.01047	-1065.00639	-1065.00580	-1064.97495	-1064.97071
ΔE	21.2	23.8	24.2	43.5	46.2
Nimag	3(71i,43i,18i)	0	3(56i,41i,16i)	0	1(119i)
Re-Re	2.623	2.871	3.116	2.925	3.002
BP86/SDD					
E	-1063.95435	-1063.93836	-1063.93801		
ΔE	13	23.1	23.3		
Nimag	1(58*i*)	0	3(51*i*,40*i*,14*i*)		
Re-Re	2.691	2.888	3.161		

Table S8. The infrared ν(CO) vibrational frequencies (cm^{-1}) predicted for singlet structures of $Re_2(CO)_8$ (infrared intensities in parentheses are in km/mol, bridging ν(CO) frequencies are in **bold**).

	MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD
8S-1 (D_{2d})	2072(76), 2072(76), 2096(2717), 2096(2717), 2100(762), 2100(0), 2145(1484), 2192(0)	2077(35), 2077(35), 2100(2728), 2100(2728), 2105(721), 2106(0), 2150(1514), 2197(0)	1954(18), 1954(18), 1975(2281), 1975(2281), 1979(522), 1980(0), 2021(1349), 2061(0)
8S-2 (C_{2v})	**1962(88), 1970(847),** 2089(57), 2106(2136), 2109(0), 2115(1763), 2153(2702), 2190(11)	**1966(87), 1974(851),** 2095(68), 2112(2068), 2114(0), 2119(1733), 2158(2664), 2195(15)	**1835(66), 1841(640),** 1967(2), 1983(1774), 1988(0), 1993(1423), 2030(2268), 2060(2)
8S-3 (C_s)	**1921(494),** 2064(376), 2077(509), 2095(1014), 2097(2022), 2127(970), 2153(2100), 2197(235)	**1924(488),** 2068(390), 2083(516), 2100(1011), 2102(1973), 2132(919), 2157(2096), 2201(225)	**1793(358),** 1929(345), 1957(437), 1975(697), 1978(1671), 2000(783), 2029(1819), 2065(203)
8S-4 (C_{2v})	**1930(476), 2057(577),** 2079(0), 2093(2460), 2108(31), 2113(1649), 2153(2571), 2190(1)	**1931(468), 2060(602),** 2086(0), 2099(2419), 2113(24), 2118(1603), 2157(2546), 2194(1)	**1794(354), 1911(456),** 1961(0), 1975(2057), 1984(36), 1989(1303), 2029(2177), 2059(1)
8S-5 (C_{2h})	2062(0), 2066(0), 2068(2196), 2080(982), 2099(0), 2110(2994), 2145(1602), 2197(0)	2068(0), 2069(0) 2073(2182), 2085(926), 2104(0), 2114(2956), 2149(1619), 2201(0)	1945(0), 1950(0), 1955(1773), 1961(829), 1977(0), 1984(2443), 2022(1410), 2067(0)
8S-6 (C_{2h})	**1985(0), 1996(1152),** 2088(0), 2092(2581), 2109(0), 2112(1632), 2152(2559), 2187(0)	**1988(0), 1998(1148),** 2094(0), 2098(2531), 2114(0), 2117(1606), 2156(2529), 2191(0)	**1842(0), 1857(878),** 1967(0), 1971(2184), 1987(0), 1988(1263), 2030(2151), 2058(0)
8S-7 (C_s)	2028(738), 2041(1008), 2094(1008), 2112(2091), 2113(1767), 2138(478), 2142(288), 2215(145)	2033(733), 2044(1009), 2100(994), 2115(2078), 2116(1731), 2141(481), 2146(266), 2219(145)	1918(953), 1919(517), 1977(911), 1992(1642), 1994(1522), 2010(414), 2020(180), 2088(134)
8S-8 (D_{2h})	2066(0), 2070(2390), 2071(0), 2091(731), 2100(0), 2114(3021), 2154(1330), 2198(0)	2071(0), 2073(0), 2075(2366), 2086(673), 2106(0), 2117(2979), 2157(1367), 2202(0)	1948(0), 1952(0), 1954(1957), 1962(533), 1981(0), 1987(2463), 2031(1133), 2068(0)
8S-9 (D_{4d})	2040(0), 2040(0), 2088(3740), 2088(3740), 2119(0), 2119(0), 2161(277), 2208(0)	2042(0), 2042(0), 2090(3701), 2090(3701), 2122(0), 2122(0), 2164(270), 2212(0)	
8S-10 (C_{2v})	2050(1459), 2062(419), 2093(480), 2102(1714), 2110(2820), 2125(0), 2140(1066), 2207(117)	2055(1436), 2065(428), 2099(455), 2105(1703), 2114(2776), 2129(0), 2144(1059), 2212(123)	

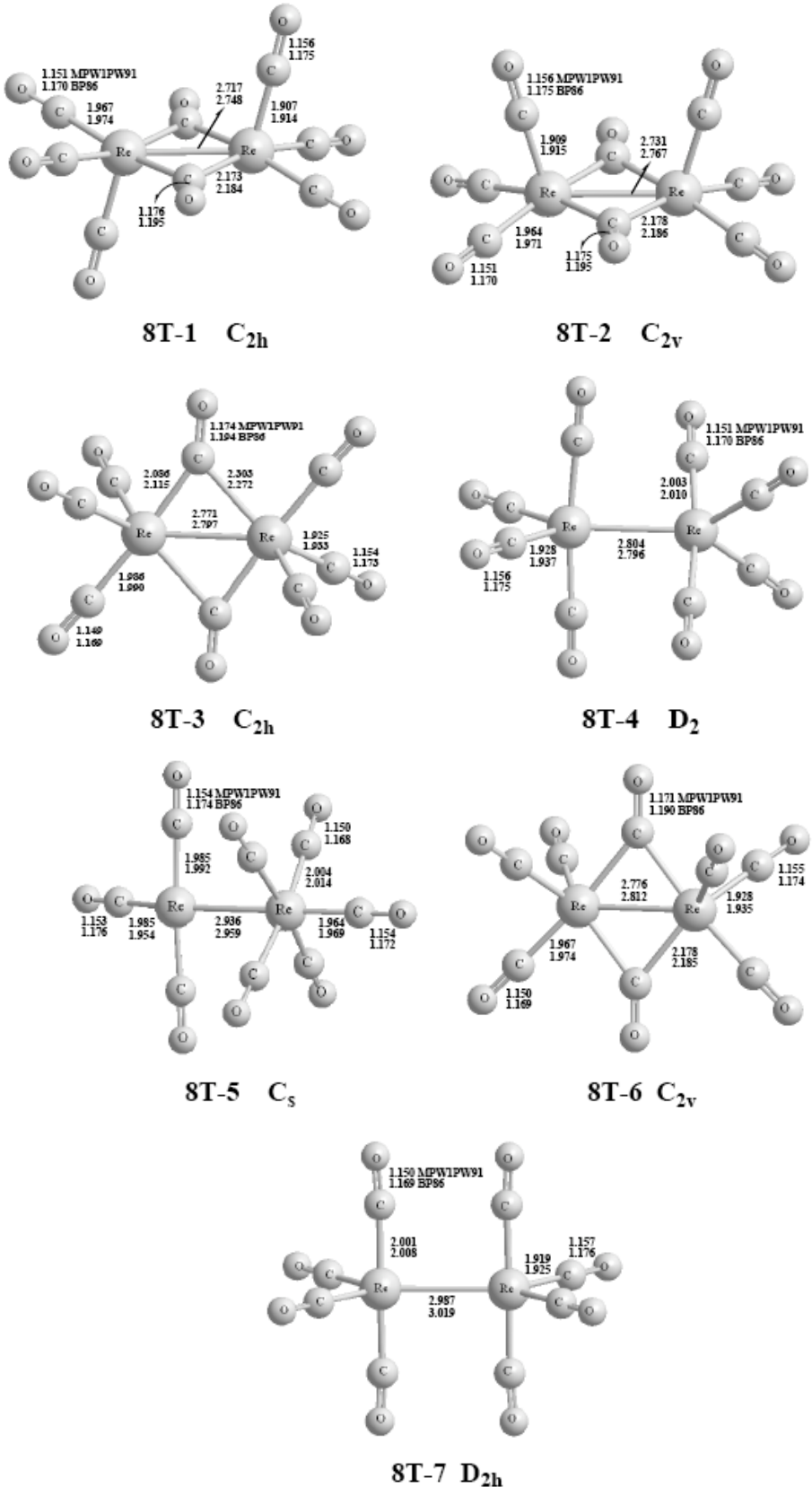

Figure S5. The optimized triplet structures of $Re_2(CO)_8$ by SDD basis sets.

Table S9. The total energies (E, in Hartree) and relative energies (ΔE, in kcal/mol) of triplet structures of $Re_2(CO)_8$. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure are also listed.

	8T-1 (C_{2h})	**8T-2** (C_{2v})	**8T-3** (C_{2h})	**8T-4** (D_2)	**8T-5** (C_s)	**8T-6** (C_{2v})	**8T-7** (D_{2h})
MPW1PW91/SDD							
E	-1063.44880	-1063.44732	-1063.44097	-1063.44043	-1063.42874	-1063.43859	-1063.43420
ΔE	20.2	21.1	25.1	25.5	32.8	26.6	29.4
Nimag	0	0	2(60i,27i)	1(23i)	0	2(92i,51i)	2(44i,30i)
Re-Re	2.717	2.731	2.771	2.804	2.936	2.776	2.987
BP86/SDD							
E	-1063.94628	-1063.94457	-1063.93975	-1063.93750	-1063.91472	-1063.93738	-1063.92856
ΔE	18.1	19.2	22.2	23.6	37.9	23.7	29.2
Nimag	0	0	2(58i,23i)	1(9i)	0	2(97i,49i)	2(43i,32i)
Re-Re	2.748	2.767	2.797	2.796	2.959	2.812	3.019

Table S10. The infrared ν(CO) vibrational frequencies (cm^{-1}) predicted for triplet structures of $Re_2(CO)_8$ (infrared intensities in parentheses are in km/mol, bridging ν(CO) frequencies are in **bold**).

	MPW1PW91/SDD	BP86/SDD
8T-1 (C_{2h})	**1892(685), 1930(0)**, 2087(0), 2093(2110), 2111(0), 2116(1867), 2145(3036), 2185(0)	**1786(550), 1809(0)**, 1969(0), 1974(1792), 1985(0), 1991(1514), 2020(2548), 2055(0)
8T-2 (C_{2v})	**1893(692), 1937(2),** 2083(46), 2098(1987), 2111(0), 2117(1871), 2147(2973), 2187(15)	**1782(555), 1809(0),** 1964(40), 1978(1660), 1987(0), 1992(1504), 2021(2524), 2056(11)
8T-3 (C_{2h})	**1911(742), 1943(0),** 2087(0), 2092(2323), 2110(0), 2113(1784), 2146(2891), 2184(0)	**1790(571), 1813(0),** 1969(0), 1974(1931), 1985(0), 1988(1453), 2022(2366), 2053(0)
8T-4 (D_2)	2070(547), 2070(157), 2084(1016), 2085(2023), 2097(0), 2106(2816), 2136(2172), 2193(0)	1947(193), 1950(113), 1962(1951), 1962(818), 1971(0), 1977(2310), 2010(1729), 2058(0)
8T-5 (C_s)	2048(689), 2074(1250), 2099(475), 2104(1771), 2111(2608), 2127(3), 2137(1037), 2209(101)	1925(747), 1934(1117), 1980(539), 1988(1520), 1992(1951), 2006(849), 2009(1), 2083(137)
8T-6 (D_{2h})	2070(0), 2074(0), 2075(2369), 2085(853), 2103(0), 2116(2999), 2150(2081), 2202(0)	1950(0), 1953(0), 1957(1963), 1962(649), 1979(0), 1988(2451), 2025(1687), 2069(0)
8S-7 (C_{2h})	2062(0), 2066(0), 2068(2196), 2080(982), 2099(0), 2110(2994), 2145(1602), 2197(0)	1945(0), 1950(0), 1955(1773), 1961(829), 1977(0), 1984(2443), 2022(1410), 2067(0)

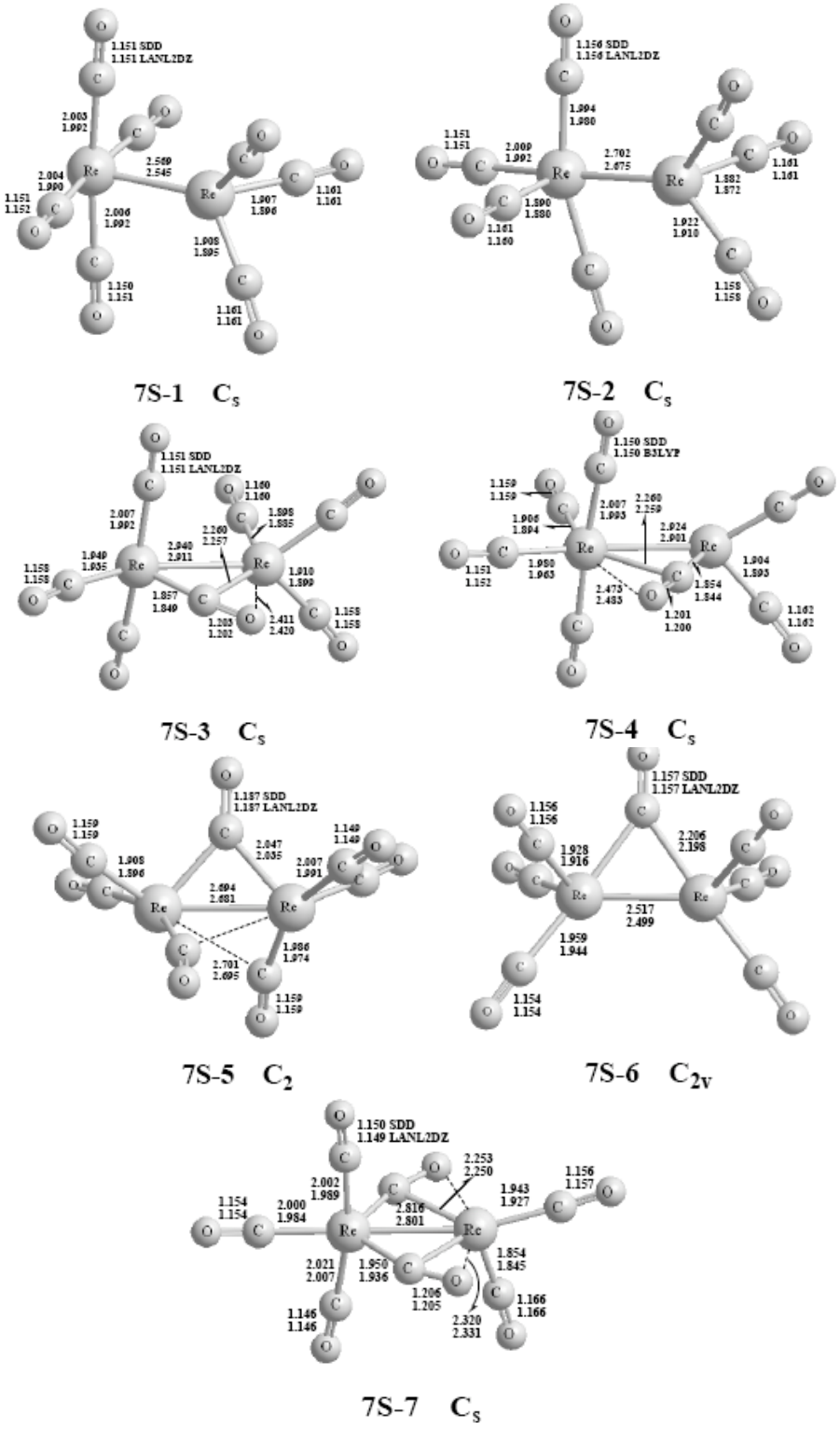

Figure S6. The optimized singlet structures of $Re_2(CO)_7$ by the MPW1PW91 method.

Table S11. The total energies (E, in Hartree) and relative energies (ΔE in kcal/mol) of $Re_2(CO)_7$. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure are also listed.

	7S-1 (C_s)	**7S-2** (C_s)	**7S-3** (C_s)	**7S-4** (C_s)	**7S-5** (C_2)	**7S-6** (C_{2v})	**7S-7** (C_s)
MPW1PW91/SDD							
E	-950.11350	-950.09884	-950.09421	-950.09120	-950.06263	-950.05973	-950.05942
ΔE	0	9.2	12.1	14	31.9	33.7	33.9
Nimag	1(8i)	0	1(4i)	0	1(27i)	2(235i,55i)	0
Re-Re	2.569	2.702	2.940	2.924	2.694	2.517	2.816
MPW1PW91/LANL2DZ							
E	-951.67520	-951.66020	-951.65500	-951.65194	-951.62227	-951.61979	-951.61769
ΔE	0	9.4	12.7	14.6	33.2	34.8	36.1
Nimag	1(6i)	0	1(4i)	0	1(26i)	2(239i,80i)	0
Re-Re	2.545	2.675	2.911	2.901	2.681	2.499	2.801
BP86/SDD							
E	-950.57557	-950.55869	-950.55686	-950.55239			
ΔE	0	10.6	11.7	14.5			
Nimag	0	0	0	0			
Re-Re	2.581	2.694	2.966	2.934			

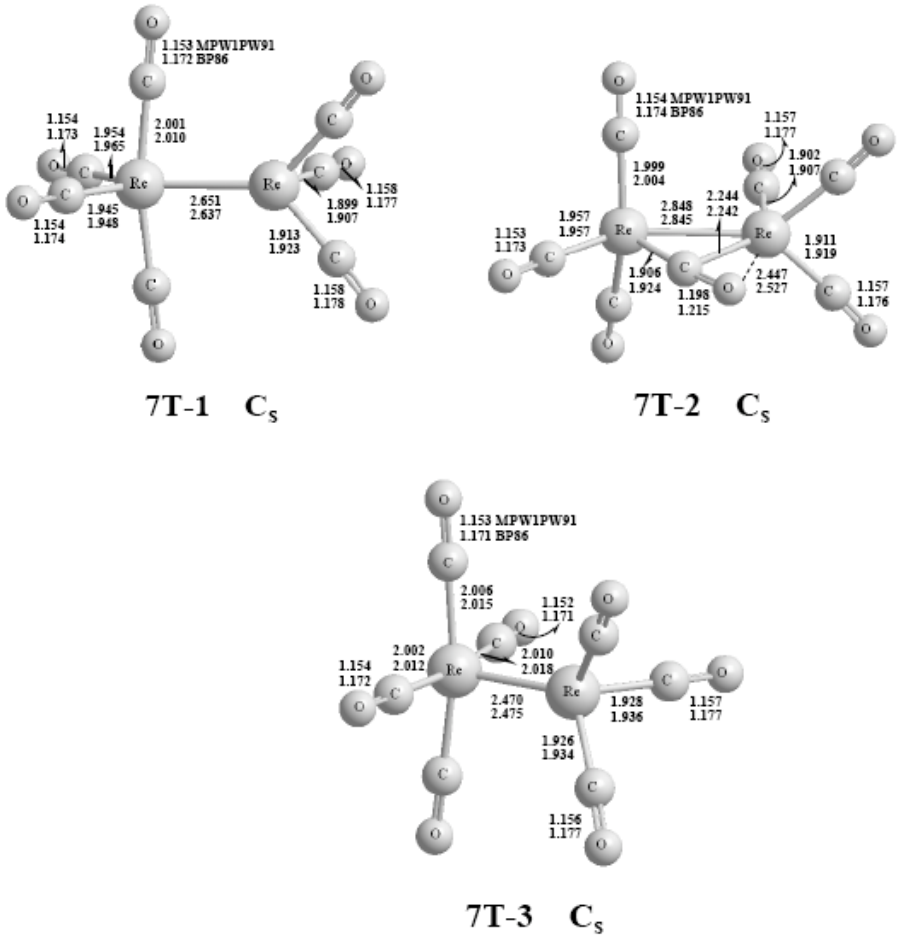

Figure S7. Three optimized triplet structures of $Re_2(CO)_7$ by SDD basis sets.

Table S12. The total energies (E, in Hartree) and relative energies (ΔE, in kcal/mol) of triplet structures of $Re_2(CO)_7$. The number of imaginary vibrational frequencies (Nimg) and the Re-Re bond distance for each structure are also listed.

		7T-1 (C_s)	**7T-2** (C_s)	**7T-3** (C_s)
MPW1PW91/ SDD	E	-950.07890	-950.07540	-950.07068
	ΔE	21.7	23.9	26.9
	Nimag	0	0	1(4i)
	Re-Re	2.651	2.848	2.470
BP86/SDD	E	-950.54255	-950.53734	-950.53631
	ΔE	20.7	24.0	24.6
	Nimag	0	0	1(7i)
	Re-Re	2.637	2.845	2.475

Table S13. The infrared ν(CO) vibrational frequencies (cm^{-1}) predicted for $Re_2(CO)_7$ (infrared intensities in parentheses are in km/mol, bridging ν(CO) frequencies are in **bold**).

	MPW1PW91/SDD	MPW1PW91/LANL2DZ	BP86/SDD
7S-1 (C_s)	2045(577), 2045(567), 2095(2369), 2096(2411), 2126(997), 2128(32), 2193(70)	2050(545), 2050(536), 2098(2369), 2099(2412), 2130(47), 2131(981), 2196(67)	1930(523), 1931(494), 1978(1874), 1978(1929), 2003(783), 2005(70), 2066(116)
7S-2 (C_s)	2050(7), 2052(397), 2063(1577), 2074(2727), 2095(473), 2126(2182), 2165(41)	2055(13), 2058(421), 2070(1536), 2078(2682), 2099(496), 2130(2147), 2170(31)	1930(22), 1939(397), 1952(2182), 1952(1145), 1969(589), 2001(1765), 2035(23)
7S-3 (C_s)	**1830(514),** 2058(1157), 2061(550), 2078(1314), 2099(2288), 2133(1300), 2173(85)	**1841(502),** 2064(1152), 2066(502), 2082(1303), 2102(2297), 2137(1292), 2177(74)	**1727(442),** 1943(918), 1944(328), 1955(980), 1970(2006), 2008(1172), 2042(88)
7-4 (C_s)	**1833(533),** 2039(822), 2073(980), 2092(2279), 2106(1986), 2116(492), 2188(341)	**1843(533),** 2043(801), 2079(971), 2096(2257), 2109(1979), 2120(486), 2191(337)	**1735(423),** 1920(663), 1959(821), 1971(1889), 1984(1659), 1991(384), 2060(315)
7S-5 (C_2)	**1885(508),** 2043(1009), 2045(1314), 2078(84), 2080(2531), 2131(2917), 2177(20)	**1890(504),** 2048(1008), 2050(1301), 2082(97), 2084(2500), 2134(2864), 2180(20)	
7S-6 (C_{2v})	**2049(686),** 2068(3039), 2074(0), 2080(131), 2087(1943), 2120(3173), 2173(0)	**2054(728),** 2073(2994), 2080(0), 2085(115), 2091(1889), 2124(3147), 2177(0)	
7S-7 (C_s)	**1761(589), 1801(477),** 2045(843), 2099(2135), 2114(796), 2132(1530), 2197(280)	**1750(591), 1788(471),** 2039(849), 2094(2215), 2108(800), 2129(1527), 2193(296)	
7T-1 (C_s)	2053(329), 2062(707), 2082(1644), 2086(2470), 2091(619), 2124(2044), 2170(75)		1930(247), 1942(447), 1957(1505), 1961(2007), 1966(404), 1996(1681), 2036(72)
7T-2 (C_s)	**1828(437),** 2064(19), 2075(807), 2078(2858), 2088(742), 2127(1910), 2163(134)		**1731(326),** 1939(337), 1954(410), 1955(1995), 1963(787), 1998(1706), 2032(140)
7T-3 (C_s)	2056(232), 2056(185), 2087(1953), 2088(2718), 2090(720), 2129(1339), 2179(49)		1931(299), 1931(271), 1966(2082), 1967(2131), 1974(21), 2002(916), 2052(146)

Complete Gaussian 03 reference (Reference 30)

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian 03, Revision C.02; Gaussian, Inc., Wallingford CT, **2004**.