Binuclear Nickel Carbonyls with the Small Bite Chelating Diphosphine Ligands Methylaminobis(difluorophosphine) and Methylenebis(dimethylphosphine): Formation of Ni=Ni Double Bonds in Preference to Ligand Cleavage

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Supporting Information

Tables S1 to S4. The ν(CO) vibrational frequencies (cm^{-1}) for the $[MeN(PF_2)_2]Ni_2(CO)_n$ (n = 6, 5, 4), $[MeN(PF_2)_2]_2Ni_2(CO)_n$ (n = 4, 3, 2), $[(Me_2P)_2CH_2]Ni_2(CO)_n$ (n = 6, 5, 4), and $[(Me_2P)_2CH_2]_2Ni_2(CO)_n$ (n = 4, 3, 2) singlet structures at the M06-L/TZP level.

Tables S5 to S8. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the singlet and triplet sturctures of $[MeN(PF_2)_2]Ni_2(CO)_n$ (n = 6, 5, 4), $[MeN(PF_2)_2]_2Ni_2(CO)_n$ (n = 4, 3, 2), $[(Me_2P)_2CH_2]Ni_2(CO)_n$ (n = 6, 5, 4), and $[(Me_2P)_2CH_2]_2Ni_2(CO)_n$ (n = 4, 3, 2) singlet and triplet structures at BP86/DZP and B3LYP/DZP levels.

Tables S9 to S20. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP level for the singlet structures of $[MeN(PF_2)_2]Ni_2(CO)_n$ (n = 6, 5, 4), $[MeN(PF_2)_2]_2Ni_2(CO)_n$ (n = 4, 3, 2), $[(Me_2P)_2CH_2]Ni_2(CO)_n$ (n = 6, 5, 4), and $[(Me_2P)_2CH_2]_2Ni_2(CO)_n$ (n = 4, 3, 2).

Tables S21 to S33. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/DZP levels of the theory for the singlet and triplet structures of $[MeN(PF_2)_2]Ni_2(CO)_n$ (n = 6, 5, 4), $[MeN(PF_2)_2]_2Ni_2(CO)_n$ (n = 4, 3, 2), $[(Me_2P)_2CH_2]Ni_2(CO)_n$ (n = 6, 5, 4), and $[(Me_2P)_2CH_2]_2Ni_2(CO)_n$ (n = 4, 3, 2).

Figures S1 to S12. Optimized singlet and triplet structures for$[MeN(PF_2)_2]Ni_2(CO)_n$ (n = 6, 5, 4), $[MeN(PF_2)_2]_2Ni_2(CO)_n$ (n = 4, 3, 2), $[(Me_2P)_2CH_2]Ni_2(CO)_n$ (n = 6, 5, 4), and $[(Me_2P)_2CH_2]_2Ni_2(CO)_n$ (n = 4, 3, 2) by the B3LYP and BP86 methods.

Table S34. Theoretical Cartesian coordinates (in Å) for the singlet structures at the M06-L/TZP level.

Table S35. Theoretical cartesian coordinates (in Å) for the singlet and triplet structures at BP86/DZP level.

Complete Gaussian 09 reference (Reference 26)

Table S1. The ν(CO) vibrational frequencies (cm^{-1}) for the $[MeN(PF_2)_2]Ni_2(CO)_n$ (n = 6, 5, 4) singlet structures at the M06-L/TZP levels (infrared intensities in parentheses are in km/mol).

	M06-L
PF-16-1S(C_1)	2085(221),2094(1378),2103(881) 2105(735),2150(370),2162(337)
PF-16-2S(C_1)	2089(778),2099(503),2102(1330) 2106(1004),2154(483),2163(214)
PF-16-3S(C_1)	2092(58),2096(1759),2098(454) 2101(1337),2152(794),2160(51)
PF-15-1S(C_1)	1971(383),2093(255),2099(1560), 2122(1025),2148(341)
PF-15-2S(C_1)	1957(425),2081(24),2104(1271) 2120(1154),2151(568)
PF-14-1S(C_S)	2002(955),2017(44),2096(1699) 2122(663)
PF-14-2S(C_S)	2107(438),2112(1365),2133(1232) 2156(31)

Table S2. The ν(CO) vibrational frequencies (cm^{-1}) for the $[MeN(PF_2)_2]_2Ni_2(CO)_n$ (n = 4, 3, 2) singlet structures at the M06-L/TZP level (infrared intensities in parentheses are in km/mol).

	M06-L
PF-24-1S(C_{2v})	2084(632),2100(470),2125(942) 2141(683)
PF-24-2S(C_S)	2085(493),2092(1078),2126(944) 2133(197)
PF-23-1S(C_1)	1958(360),2111(1059),2125(786)
PF-23-2S(C_1)	2094(834),2100(924),2132(451)
PF-22-1S(C_1)	1959(542),2110(1042)
PF-22-2S(C_S)	1952(495),2024(341)

Table S3. The ν(CO) vibrational frequencies (cm^{-1}) for the $[(Me_2P)_2CH_2]Ni_2(CO)_n$ (n = 6, 5, 4) singlet structures at the M06-L/TZP level (infrared intensities in parentheses are in km/mol).

	M06-L
PMe-16-1S(C_1)	2057(561),2058(420),2062(1450) 2064(1454),2121(687),2126(84)
PMe-16-2S(C_1)	2052(1007),2053(629),2062(346) 2078(1676),2121(167),2130(489)
PMe-16-3S(C_2)	2056(805),2056(374),2061(776) 2062(1922),2117(721),2125(186)
PMe-15-1S(C_S)	1883(432),2034(0),2064(1454), 2079(1169),2112(693)
PMe-15-2S(C_1)	2018(1042),2059(1178),2084(618), 2101(784),2140(571)
PMe-14-1S(C_1)	1948(948),1968(79),2051(1813), 2078(811)
PMe-14-2S(C_1)	2023(402),2065(799),2072(1340), 2113(767)

Table S4. The ν(CO) vibrational frequencies (cm^{-1}) for the $[(Me_2P)_2CH_2]_2Ni_2(CO)_n$ (n = 4, 3, 2) singlet structures at the M06-L/TZP level (infrared intensities in parentheses are in km/mol).

	M06-L
PMe-24-1S(C_2)	2008(1497),2021(266),2055(528), 2072(818)
PMe-24-2S(C_{2h})	2007(0),2010(1912),2054(1263), 2058(0)
PMe-23-1S(C_1)	1877(366),2027(1233),2041(845)
PMe-22-1S(C_1)	1862(443),2026(1079)
PMe-22-2S(C_i)	1986(2131),2002(0)
PMe-22-3S(C_S)	1830(435),1918(330)

Table S5. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the singlet and triplet sturctures of $[MeN(PF_2)_2]Ni_2(CO)_n$ (n=6, 5, 4) at BP86/DZP and B3LYP/DZP levels (infrared intensities in parentheses are in km/mol).

	BP86	**B3LYP**
S-PF-16-1S(C_S)	2011(592),2015(484),2017(1104) 2018(1036),2062(551),2068(135)	2093(682),2097(670),2100(1191) 2101(1196),2150(555),2156(147),
S-PF-16-2S(C_1)	2008(35),2011(1620),2015(220) 2017(1301),2058(832),2066(28)	2089(32),2092(1897),2097(241) 2099(1544),2147(821),2154(26)
S-PF-16-3S(C_1)	2006(154),2012(1176),2019(333) 2021(1209),2058(367),2069(322)	2087(166),2094(1433),2102(358) 2104(1447),2147(360),2158(344)
S-PF-15-1S(C_1)	1890(325),2013(8),2016(1589) 2036(949),2057(321)	1972(384),2095(4),2100(1866) 2123(1042),2147(354)
S-PF-15-2S(C_1)	1881(384),2000(12),2021(1129) 2035(1111),2060(463)	1966(442),2084(12),2105(1350) 2120(1268),2148(497)
S-PF-15-1T(C_1)	1833(421),1964(724),1978(894) 2006(1100),2039(719)	1903(686),2049(1046),2056(1094) 2095(1449),2130(751)
S-PF-14-1S(C_1)	1884(385),2013(748),2024(1212) 2050(442)	1963(430),2096(964),2110(1369) 2138(456)
S-PF-14-2S(C_S)	1919(826),1937(50),2018(1466) 2039(590)	2012(992),2030(37),2101(1669) 2126(683)
S-PF-14-3S(C_1)	2015(642),2023(983),2040(1155) 2060(50)	2109(440),2114(1384),2131(1354) 2155(25)
S-PF-14-1T(C_1)	2004(268),2009(1423),2021(2054) 2048(174)	2099(833),2111(2479),2117(1036) 2151(302)
S-PF-14-2T(C_S/C_1)	1868(1051),1902(28),2002(1876) 2026(523)	1933(1470),1975(91),2088(2242) 2121(655)

Table S6. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the singlet and triplet sturctures of $[MeN(PF_2)_2]_2Ni_2(CO)_n$ (n=4, 3, 2) at BP86/DZP and B3LYP/DZP levels (infrared intensities in parentheses are in km/mol).

	BP86	**B3LYP**
S-PF-24-1S(C_{2v})	2003(489),2018(453),2038(943) 2052(579)	2085(639),2100(570),2124(1008) 2139(624)
S-PF-24-2S(C_S)	2009(166),2011(1225),2040(1101) 2045(11)	2090(424),2094(1258),2127(1164) 2133(53)
S-PF-24-1T(C_S)	1932(1021),1968(466),2003(725) 2035(691)	1997(1726),2052(356),2089(972) 2126(693)
S-PF-24-2T(C_2)	1700(330),1708(160),2017(1469) 2028(270)	1914(421),1936(861),2096(2697) 2118(170)
S-PF-23-1S(C_1)	1882(303),2026(1013),2037(604)	1968(335),2110(1192),2123(700)
S-PF-23-2S(C_S)	2014(882),2015(648),2047(491)	2094(858),2099(798),2135(564)
S-PF-23-1T(C_S)	1797(273),1962(1497),2009(791)	1857(645),2049(2102),2106(843)
S-PF-23-2T(C_S)	1823(432),1974(1147),1992(499)	1899(651),2048(921),2085(1099)
S-PF-22-1S(C_S)	1881(416),2031(846)	1971(500),2115(995)
S-PF-22-2S(C_S)	1857(430),2006(435)	1955(579),2093(561)
S-PF-22-1T(C_1)	2008(1469),2019(390)	2108(1570),2129(541)
S-PF-22-2T(C_{2v}/C_S)	1987(786),2008(1054)	2045(906),2107(1354)
S-PF-22-3T(C_S)	1988(1627),2002(112)	2060(1822),2095(518)

Table S7. Infrared active n(CO) vibrational frequencies (cm^{-1}) predicted for the singlet and triplet sturctures of $[(Me_2P)_2CH_2]Ni_2(CO)_n$ (n=6, 5, 4) at BP86/DZP and B3LYP/DZP levels (infrared intensities in parentheses are in km/mol).

	BP86	**B3LYP**
S-PMe-16-1S(C_1)	1976(421),1977(552),1981(1421) 1983(995),2029(708),2035(89)	2055(460),2057(665),2060(1721) 2063(1195),2117(712),2123(93)
S-PMe-16-2S(C_2)	1978(45),1979(950),1982(921) 1983(1466),2028(647),2036(254)	2057(46),2058(1153),2062(1107) 2062(1732),2116(622),2124(264)

S-PMe-16-3S(C_1)	1975(101),1976(1366),1983(283) 1995(1471),2032(192),2040(474)	2052(19),2054(1778),2062(300) 2077(1738),2120(183),2128(496)
S-PMe-15-1S(C_S)	1819(375),1958(3),1983(1242), 1996(1102),2024(633)	1901(444),2036(0),2063(1515), 2079(1291),2111(678)
S-PMe-15-2S(C_1)	1949(885),1981(1096),1989(579), 2008(781),2042(531)	2019(1112),2061(1276),2086(597), 2106(822),2138(608)
S-PMe-15-1T(C_1)	1791(400),1922(1222),1930(516) 1973(978),2005(912)	1865(648),1999(1935),2007(543), 2058(1219),2096(988)
S-PMe-15-2T(C_1)	1797(335),1920(969),1957(513), 1958(1596),2005(788)	1869(703),1993(1477),2038(611), 2047(2051),2095(756)
S-PMe-14-1S(C_S)	1878(828),1897(43),1978(1541), 2001(756)	1969(988),1987(43),2058(1810) 2087(873)
S-PMe-14-2S(C_1)	1956(509),1984(1245),1988(624), 2027(776)	2016(1149),2058(1235),2107(611), 2143(869)
S-PMe-14-1T(C_S/C_1)	1817(1026),1852(14),1954(1995), 1979(621)	1880(1400),1924(68),2038(2427), 2076(795)
S-PMe-14-2T(C_1)	1954(117),1963(1214),1972(1976), 2005(440)	2053(90),2058(2047),2070(2043), 2098(84)

Table S8. Infrared active ν(CO) vibrational frequencies (cm^{-1}) predicted for the singlet and triplet sturctures of $[(Me_2P)_2CH_2]_2Ni_2(CO)_n$ (n=4, 3, 2) at BP86/DZP and B3LYP/DZP levels (infrared intensities in parentheses are in km/mol).

	BP86	**B3LYP**
S-PMe-24-1S(C_{2h})	1929(0),1932(1586),1969(1240), 1972(0)	2003(0),2006(2030),2053(1339), 2057(0)
S-PMe-24-2S(C_{2v})	1937(1117),1947(222),1975(484), 1992(839)	2009(1396),2022(326),2058(531), 2077(924)
S-PMe-24-1T(C_S)	1828(1001),1886(437),1938(843), 1975(568)	1891(1746),1977(422),2013(1133), 2060(600)
S-PMe-24-2T(C_2)	1807(1138),1869(499),1936(805), 1972(584)	1863(2078),1963(546),2010(1028), 2057(610)
S-PMe-24-3T(C_{2v})	1839(39),1865(337),1882(3084), 1929(663)	1893(773),1936(518),1974(4773), 2021(683)
S-PMe-23-1S(C_S)	1796(294),1945(1034),1957(773)	1876(323),2022(1274),2037(933)
S-PMe-23-2S(C_1)	1936(831),1944(1007),1973(552)	2013(239),2022(1530),2066(767)
S-PMe-23-1T(C_1)	1739(302),1865(1280),1933(913)	1804(657),1942(1989),2016(1022)
S-PMe-23-2T(C_S)	1732(399),1874(988),1899(682)	1806(611),1944(1179),1986(1069)
S-PMe-23-3T(C_2)	1758(774),1793(41),1903(1027)	1841(1032),1871(206),1991(1327)
S-PMe-23-4T(C_2)	1860(995),1937(797),1970(699)	1903(1262),2009(1068),2057(646)
S-PMe-22-1S(C_S)	1796(374),1946(941)	1876(443),2022(1158)
S-PMe-22-2S(C_{2h})	1916(1818),1928(0)	2001(2043),2007(0)
S-PMe-22-3S(C_S)	1777(549),1819(103)	1819(421),1985(539)
S-PMe-22-1T(C_1)	1793(462),1912(1167)	1951(1010),2002(1653)

Table S9. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[MeN(PF_2)_2]Ni_2(CO)_6$.

		PF-16-1S(C_1)	**PF-16-2S(C_1)**	**PF-16-3S(C_1)**
M06-L	E	-4873.918782	-4873.917518	-4873.915129
	ΔE	0.0	0.8	2.3
	Nimg	0	0	0

Table S10. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[MeN(PF_2)_2]Ni_2(CO)_5$.

		PF-15-1S(C_1)	**PF-15-2S(C_1)**
M06-L	E	-4760.551503	-4760.549726
	ΔE	0.0	1.1
	Nimg	0	0

Table S11. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[MeN(PF_2)_2]Ni_2(CO)_4$.

		PF-14-1S(C_S)	**PF-14-2S(C_S)**
M06-L	E	-4647.172717	-4647.150181
	ΔE	0.0	14.2
	Nimg	0	0

Table S12. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[MeN(PF_2)_2]_2Ni_2(CO)_4$.

		PF-24-1S(C_{2v})	**PF-24-2S(C_S)**
M06-L	E	-5824.253487	-5824.251143
	ΔE	0.0	1.5
	Nimg	0	0

Table S13. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[MeN(PF_2)_2]_2Ni_2(CO)_3$.

		PF-23-1S(C_1)	**PF-23-2S(C_1)**
M06-L	E	-5710.894199	-5710.881419
	ΔE	0.0	8.0
	Nimg	0	0

Table S14. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[MeN(PF_2)_2]_2Ni_2(CO)_2$.

		PF-22-1S(C_1)	**PF-22-2S(C_S)**
M06-L	E	-5597.500122	-5597.465025
	ΔE	0.0	22.0
	Nimg	0	0

Table S15. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[(Me_2P)_2CH_2]Ni_2(CO)_6$.

		PMe-16-1S(C_1)	**PMe-16-2S(C_2)**	**PMe-16-3S(C_2)**
M06-L	E	-4578.645270	-4578.638259	-4578.644029
	ΔE	0.0	0.7	4.3
	Nimg	0	0	0

Table S16. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[(Me_2P)_2CH_2]Ni_2(CO)_5$.

		PMe-15-1S(C_S)	**PMe-15-2S(C_1)**
M06-L	E	-4465.272314	-4465.211037
	ΔE	0.0	38.5
	Nimg	0	0

Table S17. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[(Me_2P)_2CH_2]Ni_2(CO)_4$.

		PMe-14-1S(C_1)	**PMe-14-2S(C_1)**
M06-L	E	-4351.894095	-4351.859208
	ΔE	0.0	21.9
	Nimg	0	0

Table S18. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[(Me_2P)_2CH_2]_2Ni_2(CO)_4$.

		PMe-24-1S(C_2)	**PMe-24-2S(C_{2h})**
M06-L	E	-5233.695921	-5233.695064
	ΔE	0.0	0.5
	Nimg	0	0

Table S19. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[(Me_2P)_2CH_2]_2Ni_2(CO)_3$.

		PMe-23-1S(C_1)
M06-L	E	-5120.317484
	ΔE	0.0
	Nimg	0

Table S20. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), numbers of imaginary vibrational frequencies (Nimg) at the M06-L/TZP levels for the singlet structures of $[(Me_2P)_2CH_2]_2Ni_2(CO)_2$.

		PMe-22-1S(C_1)	**PMe-22-2S(C_i)**	**PMe-22-3S(C_S)**
M06-L	E	-5006.917775	-5006.912192	-5006.904057
	ΔE	0.0	3.5	8.6
	Nimg	0	0	0

Table S21. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet structures of $[MeN(PF_2)_2]Ni_2(CO)_6$.

		S-PF-16-1S(C_S)	**S-PF-16-2S(C_1)**	**S-PF-16-3S(C_1)**
B3LYP	E	-4874.020409	-4874.017043	-4874.015671
	ΔE	0.0	2.1	3.0
	Nimg	0	0	0
BP86	E	-4874.569055	-4874.566945	-4874.564448
	ΔE	0.0	1.3	2.8
	Nimg	1(10*i*)[a]	0	0

[a]The imaginary frequency was reduced to 0*i* by using the larger (120,974) integration.

Table S22. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[MeN(PF_2)_2]Ni_2(CO)_5$.

		S-PF-15-1S(C_1)	**S-PF-15-2S(C_1)**	**S-PF-15-1T(C_1)**
B3LYP	E	-4760.661624	-4760.659578	-4760.594106
	ΔE	0.0	1.3	42.4
	$<S^2>$	0.00	0.00	2.01
	Nimg	0	0	0
BP86	E	-4761.212952	-4761.210945	-4761.136340
	ΔE	0.0	1.3	48.1
	$<S^2>$	0.00	0.00	2.00
	Nimg	0	0	0

Table S23. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[MeN(PF_2)_2]Ni_2(CO)_4$.

		S-PF-14-1S (C_1)	**S-PF-14-2S (C_S)**	**S-PF-14-3S (C_1)**	**S-PF-14-1T (C_1)**	**S-PF-14-2T (C_1/C_S)**
B3LYP	E	-4647.299825	-4647.295069	-4647.264308	-4647.248514	-4647.246028
	ΔE	0.0	3.0	22.3	32.2	33.8
	$<S^2>$	0.00	0.00	0.00	2.02	2.04
	Nimg	0	0	0	0	0
BP86	E	-4647.841803	-4647.843742	-4647.813091	-4647.785916	-4647.790877
	ΔE	0.0	-1.2	18.0	35.1	30.9
	$<S^2>$	0.00	0.00	0.00	2.01	2.02
	Nimg	0	0	0	0	0

Table S24. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[MeN(PF_2)_2]_2Ni_2(CO)_4$.

		S-PF-24-1S (C_{2v})	**S-PF-24-2S (C_S)**	**S-PF-24-1T (C_S)**	**S-PF-24-2T (C_2)**
B3LYP	E	-5824.350263	-5824.347398	-5824.270582	-5824.257176
	ΔE	0.0	1.8	48.2	58.4
	$<S^2>$	0.00	0.00	2.01	2.05
	Nimg	(4*i*)[a]	0	0	0
BP86	E	-5824.925678	-5824.924478	-5824.838156	-5824.841882
	ΔE	0.0	0.8	54.2	52.6
	$<S^2>$	0.00	0.00	2.00	2.00
	Nimg	(7*i*)[a]	0	0	0

[a]The imaginary frequencies were reduced to 0*i* by using the larger (120,974) integration.

Table S25. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[MeN(PF_2)_2]_2Ni_2(CO)_3$.

		S-PF-23-1S(C_1)	**S-PF-23-2S(C_S)**	**S-PF-23-1T(C_S)**	**S-PF-23-2T(C_S)**
B3LYP	E	-5711.001291	-5710.982539	-5710.931990	-5710.931990
	Δ E	0.0	11.8	43.5	51.1
	$<S^2>$	0.00	0.00	2.01	2.01
	Nimg	0	0	0	0
BP86	E	-5711.580260	-5711.558505	-5711.502833	-5711.492177
	Δ E	0.0	13.7	48.6	55.3
	$<S^2>$	0.00	0.00	2.00	2.00
	Nimg	0	0	0	0

Table S26. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[MeN(PF_2)_2]_2Ni_2(CO)_2$.

		S-PF-22-1S (C_S)	**S-PF-22-2S (C_S)**	**S-PF-22-1T (C_1)**	**S-PF-22-2T (C_S/C_{2v})**	**S-PF-22-3T (C_S)**
B3LYP	E	-5597.626465	-5597.587223	-5597.582033	-5597.578081	-5597.571840
	Δ E	0.0	24.6	27.9	30.4	33.2
	$<S^2>$	0.00	0.00	2.03	2.01	2.01
	Nimg	0	0	0	0	0
BP86	E	-5598.195364	-5598.157719	-5598.145820	-5598.137038	-5598.133147
	Δ E	0.0	23.6	30.1	36.6	37.8
	$<S^2>$	0.00	0.00	2.01	2.00	2.00
	Nimg	0	0	0	1(7*i*)[a]	0

[a]The imaginary frequency was reduced to 3*i* by using the larger (120,974) integration.

Table S27. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet structures of $[(Me_2P)_2CH_2]Ni_2(CO)_6$.

Singlet		**S-PMe-16-1S(C_1)**	**S-PMe-16-2S(C_2)**	**S-PMe-16-3S(C_1)**
B3LYP	E	-4578.739156	-4578.735244	-4578.734566
	ΔE	0.0	2.4	2.8
	Nimg	0	0	0
BP86	E	-4579.283529	-4579.279654	-4579.277132
	ΔE	0.0	2.4	4.0
	Nimg	0	0	0

Table S28. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[(Me_2P)_2CH_2]Ni_2(CO)_5$.

		S-PMe-15-1S (C_S)	**S-PMe-15-2S (C_1)**	**S-PMe-15-1T (C_1)**	**S-PMe-15-2T (C_1)**
B3LYP	E	-4465.373091	-4465.856055	-4465.313238	-4465.309235
	ΔE	0.0	2.8	37.6	40.1
	$<S^2>$	0.00	0.00	2.01	2.01
	Nimg	0	0	0	0
BP86	E	-4465.918543	-4465.306710	-4465.849395	-4465.847023
	ΔE	0.0	4.0	42.0	43.4
	$<S^2>$	0.00	0.00	2.00	2.00
	Nimg	0	0	0	0

Table S29. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[Me_2P)_2CH_2]Ni_2(CO)_4$.

		S-PMe-14-1S (C_S)	**S-PMe-14-2S (C_1)**	**S-PMe-14-1T (C_1/C_S)**	**S-PMe-14-2T (C_1)**
B3LYP	E	-4352.009995	-4351.966653	-4351.966533	-4351.950329
	ΔE	0.0	27.2	27.3	37.4
	$<S^2>$	0.00	0.00	2.03	2.03
	Nimg	0	0	0	0
BP86	E	-4352.553569	-4352.504555	-4352.505279	-4352.482065
	ΔE	0.0	29.8	30.3	44.9
	$<S^2>$	0.00	0.00	2.01	2.01
	Nimg	0	0	0	0

Table S30. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[Me_2P)_2CH_2]_2Ni_2(CO)_4$.

		S-PMe-24-1S (C_{2h})	**S-PMe-24-2S (C_{2v})**	**S-PMe-24-1T (C_S)**	**S-PMe-24-2T (C_2)**	**S-PMe-24-3T (C_{2v})**
B3LYP	E	-5233.771956	-5233.767891	-5233.701523	-5233.699860	-5233.669294
	ΔE	0.0	2.5	44.2	45.2	64.4
	$<S^2>$	0.00	0.00	2.00	2.01	2.05
	Nimg	0	1(17i)[a]	0	0	0
BP86	E	-5234.334958	-5234.330576	-5234.252549	-5234.252321	-5234.234830
	ΔE	0.0	2.7	51.7	51.9	60.8
	$<S^2>$	0.00	0.00	2.01	2.00	2.01
	Nimg	0	1(13i)[a]	0	0	0

[a]The imaginary frequencies were reduced to 0*i* by using the larger (120,974) integration.

Table S31. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet structures of $[Me_2P)_2CH_2]_2Ni_2(CO)_3$.

Singlet		**S-PMe-23-1S(C_S)**	**S-PMe-23-2S(C_1)**
B3LYP	E	-5120.402662	-5120.397945
	ΔE	0.0	3.0
	Nimg	1(4*i*) [a]	0
BP86	E	-5120.968010	-5120.947920
	ΔE	0.0	12.6
	Nimg	1(9*i*) [a]	0

[a]The imaginary frequencies were reduced to 0*i* by using the larger (120,974) integration.

Table S32. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the triplet structures of $[Me_2P)_2CH_2]_2Ni_2(CO)_3$.

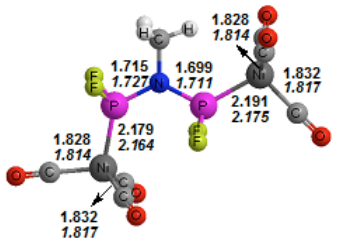
Triplet		**S-PMe-23-1T (C_1)**	**S-PMe-23-2T (C_S)**	**S-PMe-23-3T (C_2)**	**S-PMe-23-4T (C_2)**
B3LYP	E	-5120.346014	-5120.344488	-5120.340126	-5120.338923
	ΔE	35.5	36.5	39.2	40.0
	$<S^2>$	2.01	2.01	2.01	2.01
	Nimg	0	0	0	0
BP86	E	-5120.903083	-5120.901198	-5120.898233	-5120.882803
	ΔE	40.7	41.9	43.8	53.5
	$<S^2>$	2.00	2.00	2.00	2.00
	Nimg	0	0	0	0

Table S33. Total energies (E, in hartree), relative energies (ΔE, in kcal/mol), spin square values $<S^2>$, number of imaginary vibrational frequencies (Nimg) at the B3LYP/DZP and BP86/ DZP levels of the theory for the singlet and triplet structures of $[Me_2P)_2CH_2]_2Ni_2(CO)_2$.

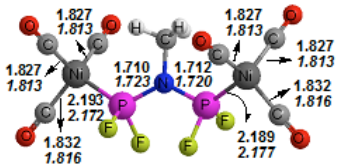
		S-PMe-22-1S (C_S)	**S-PMe-22-2S (C_{2h})**	**S-PMe-22-3S (C_S)**	**S-PMe-22-1T (C_1)**
B3LYP	E	-5007.029093	-5007.027565	-5007.006361	-5006.981137
	ΔE	0.0	1.0	14.3	29.1
	$<S^2>$	0.00	0.00	0.00	2.01
	Nimg	1(3*i*)[a]	0	0	0
BP86	E	-5007.583542	-5007.572783	-5007.564715	-5007.526292
	ΔE	0.0	6.8	11.8	35.9
	$<S^2>$	0.00	0.00	0.00	2.00
	Nimg	1(14*i*)[b]	0	0	0

[a]The imaginary frequencies were reduced to 3*i* by using the larger (120,974) integration.

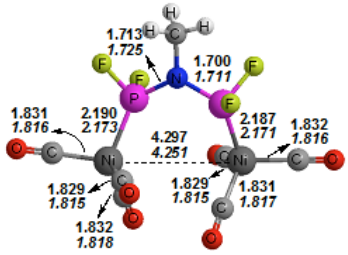
[b]The imaginary frequencies were reduced to 0*i* by using the larger (120,974) integration.



PF-16-1S(C_S,0.0,0.0)

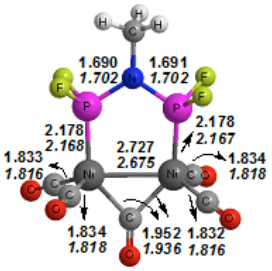


PF-16-2S(C_1,2.1,1.3)

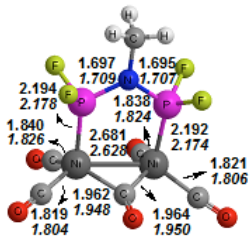


PF-16-3S(C_1,3.0,2.8)

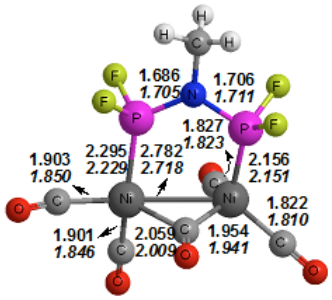
Fig.S1 The three singlet structures found for $[MeN(PF_2)_2]Ni_2(CO)_6$. The upper numbers for bond distances (Å) were obtained by the B3LYP method while the lower numbers were obtained by the BP86 method. The relative energies are shown in parentheses, predicted by the B3LYP method and the BP86 method, respectively. The data in all of the following figures in the present text have the same arrangement.



PF-15-1S（C1,0.0,0.0）

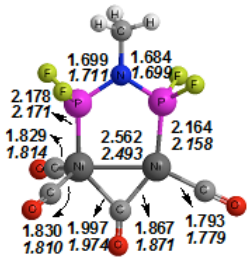


PF-15-2S(C1,1.3,1.3)

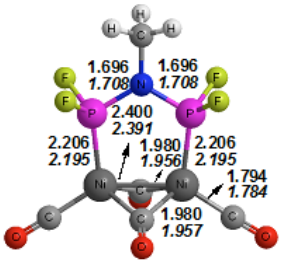


PF-15-1T(C1,42.4,48.1)

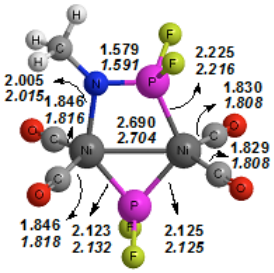
Fig.S2 The two singlet and one triplet structures found for $[MeN(PF_2)_2]Ni_2(CO)_5$.



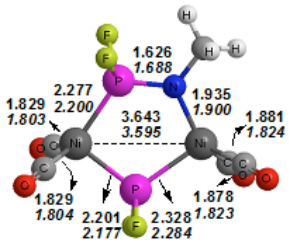
PF-14-1S(C1,0.0,0.0)



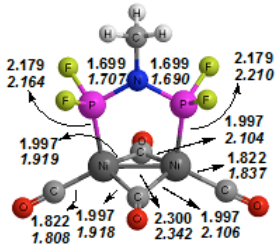
PF-14-2S(CS ,3.0,-1.2)



PF-14-3S(C_1,22.3,18.0)

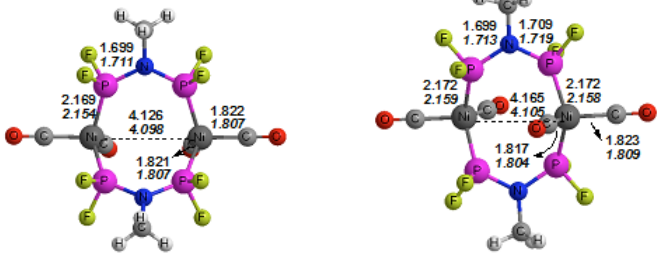


PF-14-1T(C_1,32.2,35.1)

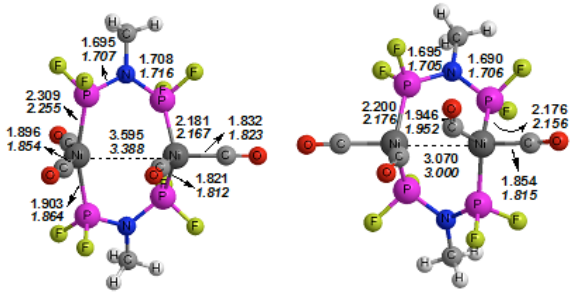


PF-14-2T(C_1/C_S,33.8.30.9)

Fig.S3 The three singlet and two triplet structures found for $[MeN(PF_2)_2]Ni_2(CO)_4$.

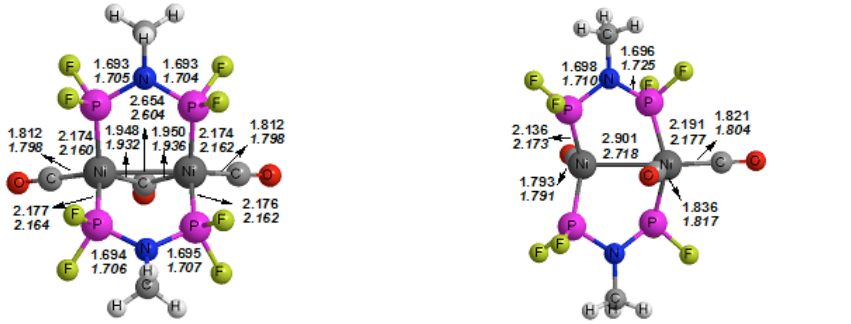


S-PF-24-1S(C_{2V}, 0.0,0.0) **S-PF-24-2S(C_S,1.8,0.8)**

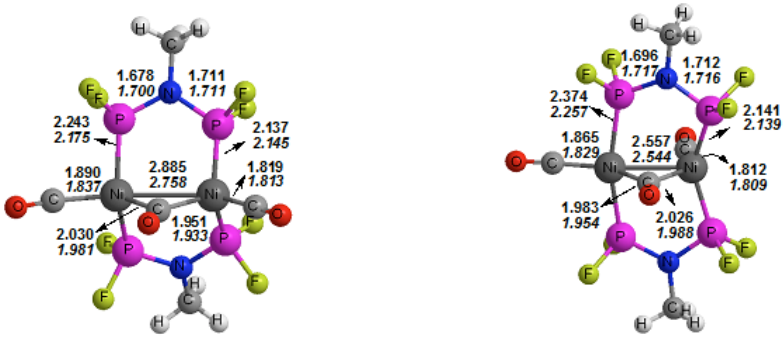


S-PF-24-1T(C_S,48.2,54.2) **S-PF-24-2T(C_2,58.4,52.6)**

Fig.S4 The two singlet and two triplet structures found for $[MeN(PF_2)_2]_2Ni_2(CO)_4$.

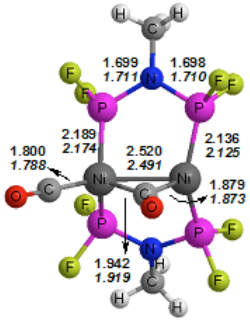


S-PF-23-1S(C_1,0.0,0.0) **S-PF-23-2S(C_S,11.8,15.5)**

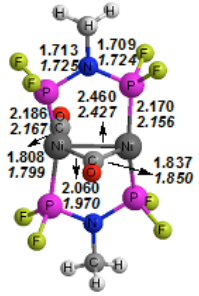


S-PF-23-1T(C_S,43.5,48.6) **S-PF-23-2T(C_S,55.1,55.3)**

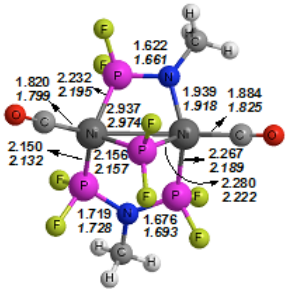
Fig.S5 The two singlet and two triplet structures found for $[MeN(PF_2)_2]_2Ni_2(CO)_3$.



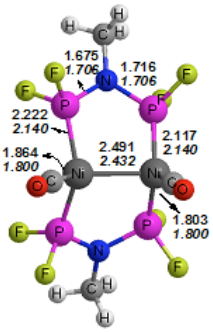
S-PF-22-1S(C_S,0.0,0.0)



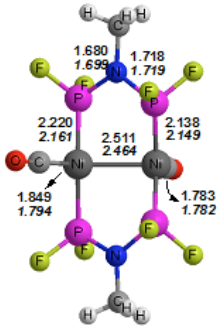
S-PF-22-2S(C_S,24.6,23.6)



S-PF-22-1T(C_S,27.9,30.1)

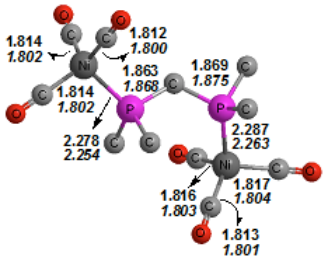


S-PF-22-2T(C_S/C_{2v},30.4,36.6)

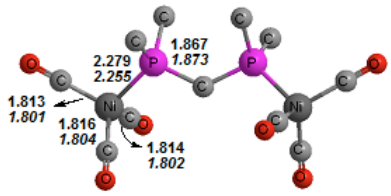


PF-22-3T(C_S,33.2,37.8)

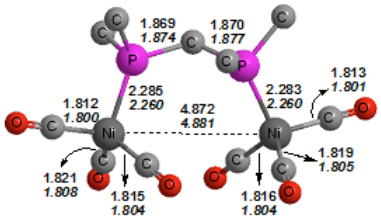
Fig.S6 The two singlet and three triplet structures found for $[MeN(PF_2)_2]_2Ni_2(CO)_2$.



S-PMe-16-1S(C_1,0.0,0.0)

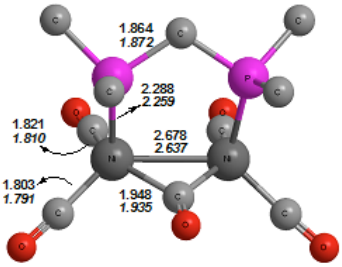


S-PMe-16-2S(C_2,2.4,2.4)

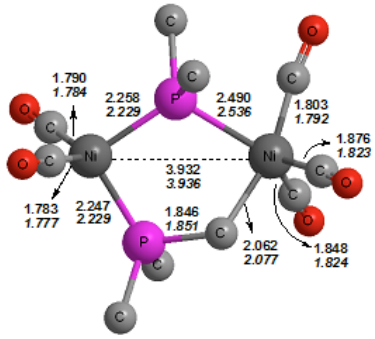


S-PMe-16-3S(C_1,2.8,4.0)

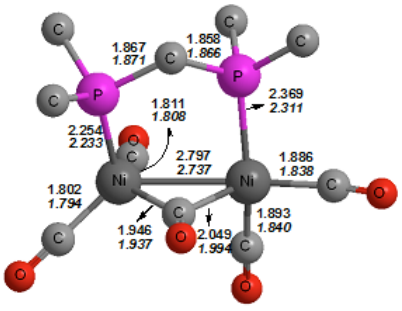
Fig.S7 The three singlet structures found for $[(Me_2P)_2CH_2]Ni_2(CO)_6$.



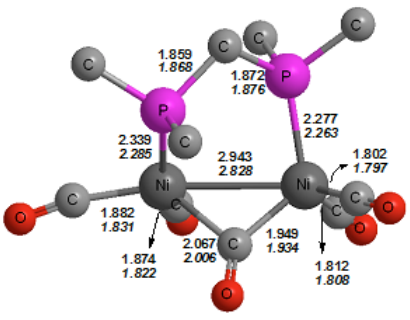
S-PMe-15-1S(C_S,0.0,0.0)



S-PMe-15-2S(C_1,2.8,4.0)

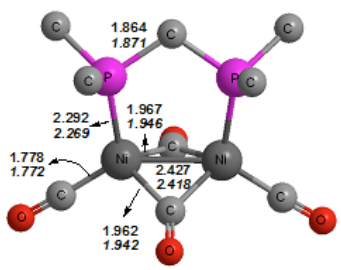


S-PMe-15-1T(C_1,37.6,42.0)

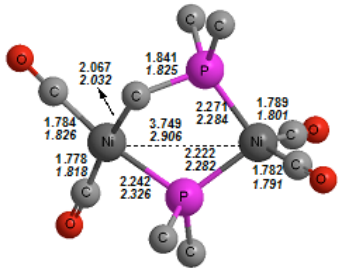


S-PMe-15-2T(C_1,40.1,43.4)

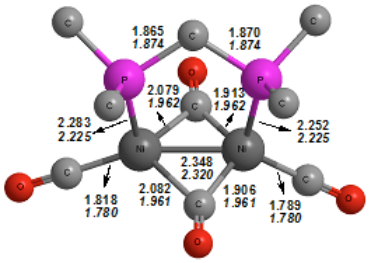
Fig.S8 The two singlet and two triplet structures found for $[(Me_2P)_2CH_2]Ni_2(CO)_5$.



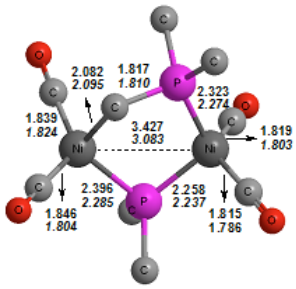
S-PMe-14-1S(C_S,0.0,0.0)



S-PMe-14-2S(C_1,27.2,29.8)

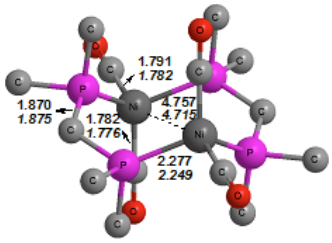


S-PMe-14-1T(C_1/C_S,27.3,30.3)

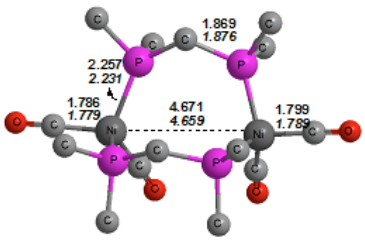


S-PMe-14-2T(C_1,37.4,44.9)

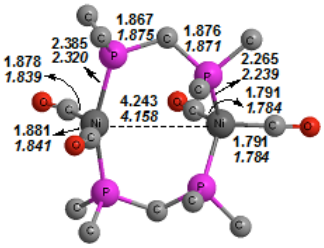
Fig.S9 The two singlet and two triplet structures found for $[(Me_2P)_2CH_2)]Ni_2(CO)_4$.



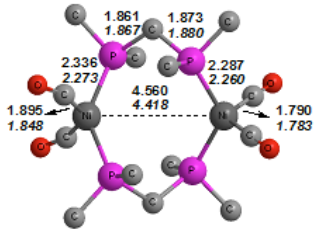
S-PMe-24-1S(C_{2h},0.0,0.0)



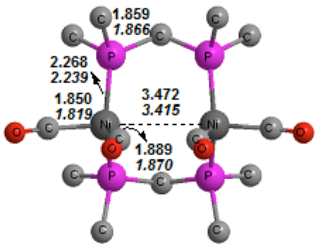
S-PMe-24-2S(C_{2v},2.5,2.7)



S-PMe-24-1T(C_S,44.2,51.7)

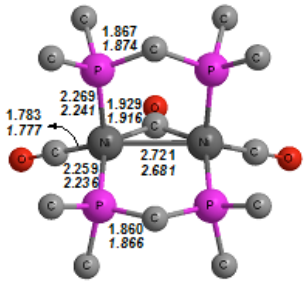


S-PMe-24-2T(C_2,45.2,51.9)

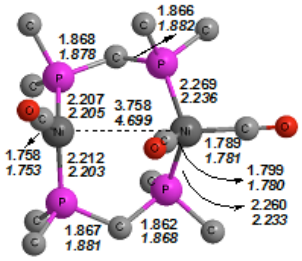


S-PMe-24-3T(C_{2v},64.4,60.8)

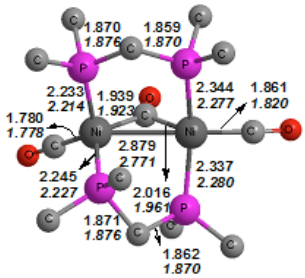
Fig.S10 The two singlet and three triplet structures found for $[(Me_2P)_2CH_2]_2Ni_2(CO)_4$.



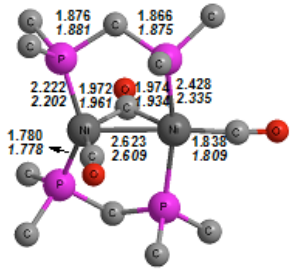
S-PMe-23-1S(C_S,0.0,0.0)



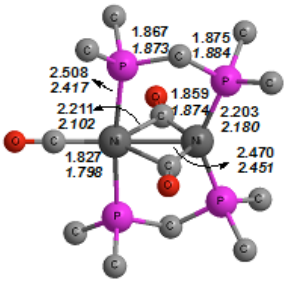
S-PMe-23-2S(C_1,3.0,12.6)



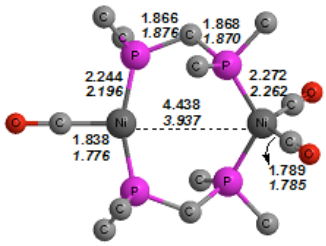
S-PMe-23-1T(C_1,35.5,40.7)



S-PMe-23-2T(C_S,36.5,41.9)

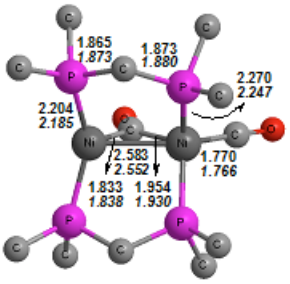


S-PMe-23-3T(C_1,39.2,43.8)

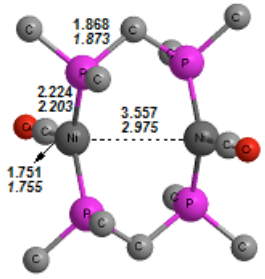


S-PMe-23-4T(C_S,40.0,53.5)

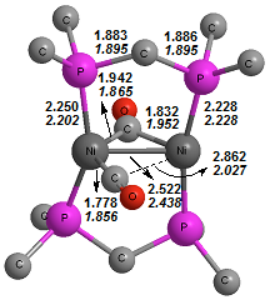
Fig.S11 The two singlet and four triplet structures found for $[(Me_2P)_2CH_2]_2Ni_2(CO)_3$.



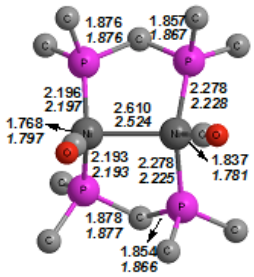
S-PMe-22-1S(C_S,0.0,0.0)



S-PMe-22-2S(C_1,1.0,6.8)



S-PMe-22-3S(C_S,14.3,11.8)



S-PMe-22-1T(C_1,29.1,35.9)

Fig.S12 The three singlet and one triplet structure found for $[(Me_2P)_2CH_2]_2Ni_2(CO)_2$.

Table S34. Theoretical Cartesian coordinates (in Å) for the structures at M06-L/TZP level.

Structures	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
PF-16-1S(C_1)	7	-0.022318	2.041145	0.046855
	6	-0.086315	3.513255	0.140369
	1	0.854707	3.890069	0.530202
	1	-0.254025	3.952985	-0.842725
	1	-0.888419	3.816883	0.809545
	15	-1.361243	1.191049	-0.565008
	15	1.420725	1.254968	0.438099
	9	-1.185855	1.430277	-2.127994
	9	2.436400	2.345361	-0.122959
	9	-2.425584	2.351743	-0.354556
	9	1.573158	1.699063	1.956618
	28	-2.047761	-0.690624	0.211350
	28	1.995400	-0.729141	-0.162545
	6	-1.465376	-0.722104	1.927817
	6	3.808420	-0.664541	-0.117904
	6	-3.856949	-0.581863	0.116236
	6	1.414520	-0.985766	-1.861190
	8	-1.087784	-0.706190	3.004998
	8	4.948364	-0.635113	-0.096076
	8	-4.994246	-0.517113	0.060198
	8	1.072534	-1.150234	-2.937415
	6	1.412078	-2.036012	0.956903
	8	1.072266	-2.881627	1.643751
	6	-1.481983	-2.137944	-0.732001
	8	-1.140084	-3.063842	-1.304116
PF-16-2S(C_1)	7	0.092839	-1.178869	0.025546
	6	0.792061	-2.473305	-0.050682
	1	1.811379	-2.356133	0.313975
	1	0.284480	-3.202084	0.578252
	1	0.822905	-2.847508	-1.074500
	15	-1.610185	-1.209843	0.042850
	15	1.017929	0.233069	0.029162
	9	-1.817163	-2.227329	1.248457
	9	-1.818435	-2.301848	-1.096275
	9	0.319605	1.062757	-1.133171

	9	0.323182	1.038146	1.209789
	28	3.163643	0.151582	-0.002786
	28	-2.916528	0.479581	-0.012987
	6	-2.630606	1.387866	-1.558224
	6	-2.616438	1.539309	1.430561
	6	-4.588065	-0.218646	0.038154
	6	3.746569	-0.557208	1.559028
	6	3.721342	1.869362	-0.191128
	6	3.654340	-0.867813	-1.416751
	8	-2.450760	1.960642	-2.527874
	8	-2.437642	2.207454	2.337149
	8	-5.643041	-0.652741	0.068844
	8	4.077525	2.945948	-0.311287
	8	4.112136	-1.009705	2.541276
	8	3.948787	-1.524858	-2.303112
	7	-0.007186	0.009995	-0.016230
	6	-0.020357	1.477763	-0.102531
	1	-0.777297	1.894123	0.562507
	1	0.952112	1.861647	0.202341
	1	-0.215876	1.821984	-1.120417
	15	-1.503196	-0.769589	-0.242562
	15	1.488508	-0.759153	0.228017
	9	1.254551	-2.066332	-0.629740
	9	-1.307606	-1.423846	-1.673827
	9	1.267995	-1.451829	1.636506
	9	-1.232540	-2.086442	0.584942
	28	3.338200	0.303526	-0.048975
PF-16-3S(C_1)	28	-3.337301	0.300314	0.074217
	6	3.206930	1.234666	-1.597247
	8	3.104491	1.824231	-2.569995
	6	4.625747	-0.972180	-0.138524
	6	3.608607	1.396230	1.369843
	6	-4.678788	-0.894143	-0.185679
	6	-3.405059	1.647943	-1.131539
	6	-3.328828	0.931814	1.772020
	8	5.437617	-1.771243	-0.191973
	8	3.776462	2.085805	2.264214
	8	-3.318375	1.337527	2.839261
	8	-3.424746	2.500767	-1.891051
	8	-5.526022	-1.639664	-0.350258

PF-15-1S(C_1)	7	-0.061973	2.252988	-0.026276
	6	-0.108014	3.716918	0.015474
	1	0.837469	4.119582	-0.342618
	1	-0.904432	4.077608	-0.633709
	1	-0.286501	4.070625	1.030959
	15	-1.431844	1.285477	-0.110148
	15	1.354339	1.360004	0.087377
	9	-2.130567	1.891104	-1.403309
	9	-2.359332	2.069471	0.917608
	9	2.003976	2.017259	1.381867
	9	2.258506	2.174242	-0.937518
	28	-1.290618	-0.840044	0.104112
	28	1.332443	-0.772297	-0.105927
	6	-1.854246	-1.146199	1.804689
	6	-2.353959	-1.458643	-1.226974
	6	0.055698	-2.232090	-0.035169
	6	1.988902	-1.058859	-1.775285
	6	2.369179	-1.328431	1.273977
	8	-3.058837	-1.809813	-2.052336
	8	-2.236656	-1.311176	2.866780
	8	0.083551	-3.390320	-0.057928
	8	3.058027	-1.642050	2.127517
	8	2.433931	-1.209173	-2.814837

PF-15-2S(C_1)	7	-0.200848	2.161860	-0.033423
	6	-0.316141	3.625491	0.017498
	1	-1.182296	3.942933	-0.560127
	1	-0.425761	3.970781	1.045598
	1	0.572146	4.077305	-0.419772
	15	-1.572710	1.186548	-0.101060
	15	1.296178	1.398832	0.110348
	9	-2.460213	1.890123	1.014461
	9	2.132556	2.286615	-0.910354
	9	-2.328361	1.871507	-1.320224
	9	1.856788	2.132467	1.406031
	28	-1.227553	-0.930184	0.001280
	28	1.371276	-0.744811	-0.056872
	6	-1.269319	-1.335490	1.775241

	6	2.763633	-1.278176	-1.068856
	6	-2.474590	-1.968073	-0.792881
	8	-1.355019	-1.577060	2.887770
	8	3.672649	-1.595170	-1.680152
	8	-3.295497	-2.607319	-1.259886
	6	1.635905	-1.480708	1.589371
	8	1.868880	-1.943152	2.606432
	6	0.055968	-1.076953	-1.462202
	8	0.032228	-1.220782	-2.613256

PF-14-1S(C_S)	7	-0.022420	2.177431	0.000000
	6	0.026391	3.642137	0.000000
	1	-0.483039	4.025213	-0.882712
	1	-0.483039	4.025213	0.882712
	1	1.057054	3.997333	0.000000
	15	-0.011053	1.280531	1.425072
	15	-0.011053	1.280531	-1.425072
	9	-1.184006	2.008667	2.212805
	9	-1.184006	2.008667	-2.212805
	9	1.159814	2.025254	2.200948
	9	1.159814	2.025254	-2.200948
	28	-0.001133	-0.878229	1.180945
	28	-0.001133	-0.878229	-1.180945
	6	0.008868	-1.845610	2.676014
	6	0.008868	-1.845610	-2.676014
	8	0.016490	-2.425058	3.661832
	8	0.016490	-2.425058	-3.661832
	6	1.435407	-1.473489	0.000000
	8	2.476147	-1.968645	0.000000
	6	-1.418012	-1.516797	0.000000
	8	-2.443206	-2.043645	0.000000

PF-14-2S(C_S)	7	-0.120821	2.111422	-0.000026
	6	-0.548829	3.482193	-0.000044
	1	-1.156889	3.706870	0.881561
	1	0.301009	4.169199	-0.000042
	1	-1.156871	3.706852	-0.881668
	15	1.273979	1.396001	-0.000014

	28	-1.230794	0.430734	-0.000003
	28	1.066329	-0.792545	0.000007
	9	2.198653	1.980962	-1.167391
	9	2.198645	1.980984	1.167359
	6	-2.102572	0.584725	1.594889
	6	-2.102592	0.584697	-1.594884
	6	1.822092	-1.305767	-1.566947
	6	1.822093	-1.305740	1.566969
	8	2.297518	-1.616272	2.554933
	8	2.297516	-1.616316	-2.554906
	8	-2.679069	0.680321	2.572634
	8	-2.679100	0.680277	-2.572624
	15	-0.850620	-1.639029	0.000012
	9	-1.427700	-2.528284	-1.174622
	9	-1.427702	-2.528269	1.174657
PF-24-1S(C_{2v})	7	2.420203	0.000000	-0.865880
	6	3.626900	0.000000	-1.719677
	1	4.225337	0.882001	-1.503714
	1	4.225337	-0.882001	-1.503714
	1	3.351534	0.000000	-2.773251
	15	1.761141	-1.493937	-0.439671
	15	1.761141	1.493937	-0.439671
	9	3.082276	-2.185645	0.119247
	9	1.847512	-2.185329	-1.872938
	9	1.847512	2.185329	-1.872938
	9	3.082276	2.185645	0.119247
	28	0.000000	-2.023033	0.643923
	28	0.000000	2.023033	0.643923
	15	-1.761141	-1.493937	-0.439671
	15	-1.761141	1.493937	-0.439671
	9	-3.082276	-2.185645	0.119247
	9	-1.847512	-2.185329	-1.872938
	9	-1.847512	2.185329	-1.872938
	9	-3.082276	2.185645	0.119247
	6	0.000000	-1.618038	2.405187
	6	0.000000	-3.818560	0.487090
	6	0.000000	3.818560	0.487090
	6	0.000000	1.618038	2.405187
	8	0.000000	-4.956919	0.401394
	8	0.000000	-1.495447	3.540228
	8	0.000000	4.956919	0.401394

	8	0.000000	1.495447	3.540228
	7	-2.420203	0.000000	-0.865880
	6	-3.626900	0.000000	-1.719677
	1	-4.225337	-0.882001	-1.503714
	1	-4.225337	0.882001	-1.503714
	1	-3.351534	0.000000	-2.773251
	7	-0.009408	2.717326	0.094332
	6	0.061028	4.180567	0.252365
	1	0.409367	4.640858	-0.671573
	1	-0.928677	4.568024	0.475091
	1	0.738407	4.451797	1.060895
	15	-1.401085	1.854218	0.506821
	15	1.349992	1.875943	-0.480267
	9	-2.476671	2.983288	0.189353
	9	-1.442599	2.070867	2.082900
	9	2.414915	3.020731	-0.191115
	9	1.251250	2.161395	-2.041435
	28	-1.926489	-0.000002	-0.431517
	28	1.978688	0.000002	0.347960
	15	-1.401081	-1.854220	0.506822
	15	1.349996	-1.875942	-0.480266
	9	-2.476665	-2.983293	0.189355
PF-24-2S(C_S)	9	-1.442593	-2.070869	2.082900
	9	2.414922	-3.020727	-0.191113
	9	1.251256	-2.161394	-2.041434
	6	-3.732669	-0.000003	-0.419280
	6	3.773390	0.000004	0.143746
	8	-4.874280	-0.000004	-0.422266
	8	4.908435	0.000004	0.020595
	7	-0.009404	-2.717326	0.094332
	6	0.061033	-4.180567	0.252364
	1	-0.928674	-4.568023	0.475088
	1	0.409372	-4.640859	-0.671573
	1	0.738410	-4.451799	1.060895
	6	-1.256914	-0.000002	-2.106544
	8	-0.881620	-0.000002	-3.185304
	6	1.441382	0.000003	2.067902
	8	1.127054	0.000003	3.166409
	7	-2.370158	-0.216937	-1.070584
PF-23-1S(C_1)	6	-3.489760	-0.324620	-2.013817

	1	-3.997074	-1.277043	-1.872363
	1	-4.203999	0.475116	-1.827034
	1	-3.138234	-0.255446	-3.043367
	15	-1.852382	1.283433	-0.501703
	15	-1.482459	-1.574759	-0.612138
	9	-3.242506	1.870025	0.005028
	9	-1.862258	2.099398	-1.866890
	9	-1.202324	-2.212100	-2.043898
	9	-2.682224	-2.562604	-0.268714
	28	-0.135853	1.279739	0.776531
	28	0.114265	-1.282453	0.784580
	15	1.574314	1.558098	-0.472448
	15	1.909152	-1.234720	-0.367674
	9	2.728429	2.526452	0.038129
	9	1.420497	2.282784	-1.882202
	9	1.985194	-2.086344	-1.710713
	9	3.242897	-1.849239	0.242892
	6	-0.035777	2.634552	1.954308
	6	0.347842	-2.635529	1.942395
	6	-0.661215	-0.063743	2.072654
	8	0.042424	3.523351	2.666303
	8	0.508580	-3.522107	2.643200
	8	-1.227231	-0.109201	3.085014
	7	2.491821	0.232404	-0.942775
	6	3.656832	0.338443	-1.824954
	1	4.158721	1.289303	-1.653554
	1	4.356756	-0.465026	-1.602345
	1	3.360196	0.273719	-2.871841
	7	-2.880579	-0.132752	-0.359087
	6	-4.262003	0.101578	-0.759928
	1	-4.306040	0.773653	-1.615867
	1	-4.714059	-0.850103	-1.035252
	1	-4.835354	0.535849	0.059566
	15	-2.036472	-1.551757	-0.163163
	15	-1.759341	0.998984	0.237601
PF-23-2S(C_1)	9	-2.238568	-2.293501	-1.553178
	9	-3.062329	-2.474374	0.621622
	9	-2.223850	1.290833	1.731436
	9	-2.582171	2.267252	-0.342980
	28	-0.219616	-0.836896	0.621758
	28	0.267990	1.481616	-0.425204
	15	1.465174	-1.774910	-0.261521

	15	2.204925	0.803479	0.178475
	9	1.490316	-2.365657	-1.737591
	9	2.145116	-3.052448	0.395498
	9	2.684564	0.927524	1.687863
	9	3.421904	1.648658	-0.412761
	6	0.234437	3.187932	0.143231
	8	0.225869	4.273683	0.492924
	7	2.765823	-0.717943	-0.281823
	6	4.163876	-1.055317	-0.541311
	1	4.236131	-2.118214	-0.763216
	1	4.545672	-0.490169	-1.390701
	1	4.780203	-0.842623	0.332578
	6	0.182928	1.163428	-2.212583
	8	0.112316	0.916965	-3.325009
	6	-0.040702	-0.830649	2.413960
	8	0.067054	-0.838027	3.551524
	7	2.352928	-1.183894	0.320058
	6	3.462875	-1.891472	0.963698
	1	3.560143	-2.886219	0.532050
	1	4.393005	-1.351489	0.792772
	1	3.296110	-1.983124	2.037050
	15	2.302143	0.498794	0.224905
	15	1.024841	-1.979752	-0.331761
	9	3.654515	0.783389	-0.563116
	9	2.912200	0.833642	1.656453
	9	0.771758	-3.042296	0.823898
	9	1.747472	-3.004276	-1.309828
	28	0.455777	1.435478	-0.374617
PF-22-1S(C_1)	28	-0.482164	-0.667876	-1.026509
	15	-0.921852	0.828415	1.181417
	15	-2.478078	-0.861741	-0.428534
	9	-1.396730	1.947654	2.216855
	9	-0.332182	-0.145223	2.308629
	9	-3.147698	-2.159564	0.207620
	9	-3.810516	-0.382164	-1.153154
	6	0.660057	3.193205	-0.561560
	6	-0.527178	0.981012	-1.960743
	8	0.806953	4.322902	-0.651214
	8	-0.971289	1.379181	-2.956826
	7	-2.453139	0.151510	0.920886
	6	-3.525088	0.205172	1.919317
	1	-3.831985	1.235519	2.090834

	1	-4.379647	-0.358644	1.550952
	1	-3.201831	-0.232551	2.864679
	7	0.033163	-0.023337	2.908172
	6	0.059803	0.001426	4.380574
	1	-0.825733	-0.493576	4.774732
	1	0.934888	-0.535943	4.740954
	1	0.091105	1.025295	4.752856
	15	1.526824	-0.026372	2.081688
	15	-1.479636	0.002435	2.135538
	9	2.210797	-1.263852	2.811868
	9	2.270834	1.082908	2.945212
	9	-2.182512	1.101843	3.046483
	9	-2.152478	-1.252102	2.841894
	28	1.100834	0.152623	0.000000
	28	-1.234189	-0.014469	0.000000
PF-22-2S(C_S)	15	1.526824	-0.026372	-2.081688
	15	-1.479636	0.002435	-2.135538
	9	2.210797	-1.263852	-2.811868
	9	2.270834	1.082908	-2.945212
	9	-2.182512	1.101843	-3.046483
	9	-2.152478	-1.252102	-2.841894
	7	0.033163	-0.023337	-2.908172
	6	0.059803	0.001426	-4.380574
	1	0.934888	-0.535943	-4.740954
	1	-0.825733	-0.493576	-4.774732
	1	0.091105	1.025295	-4.752856
	6	0.036905	-1.424332	0.000000
	8	-0.103648	-2.578380	0.000000
	6	0.220650	1.727672	0.000000
	8	-0.327485	2.742064	0.000000
	15	-1.633358	1.224214	-0.030333
	15	1.219258	-0.294585	-0.295457
	28	3.383555	0.034999	0.116948
	6	4.260480	-1.147645	-0.917893
PMe-16-1S(C_1)	6	3.582164	-0.288307	1.876113
	6	3.700036	1.747778	-0.327569
	8	4.799368	-1.905997	-1.587346
	8	3.858858	2.847830	-0.611697
	8	3.682401	-0.500158	2.998247
	28	-3.093851	-0.466398	0.079861

	6	-2.790803	-1.227498	1.684387
	6	-4.681767	0.378640	-0.034897
	6	-2.837857	-1.589845	-1.302300
	8	-2.558846	-1.695116	2.704643
	8	-5.677725	0.939263	-0.114982
	8	-2.678629	-2.305994	-2.183768
	6	0.512259	-1.827148	0.387930
	1	-0.546865	-1.938528	0.154993
	1	1.058760	-2.676987	-0.021206
	1	0.642580	-1.839396	1.470475
	6	0.729613	-0.395310	-2.049103
	1	1.295658	-1.198149	-2.521858
	1	-0.334492	-0.602944	-2.173871
	1	0.981832	0.532097	-2.563581
	6	0.147571	1.024596	0.414316
	1	0.647884	1.981440	0.233179
	1	0.185300	0.871371	1.497770
	6	-2.058775	2.584225	1.114702
	1	-1.357460	3.417013	1.033845
	1	-3.062809	2.945153	0.890510
	1	-2.056864	2.219852	2.141633
	6	-1.567997	2.138836	-1.610154
	1	-2.552145	2.572207	-1.791624
	1	-0.831461	2.944681	-1.583424
	1	-1.343078	1.478383	-2.444610

	28	2.385459	-0.579530	-0.135889
	28	-2.203077	-0.712800	0.144820
	6	3.909368	-0.151957	-0.987052
	6	2.667922	-1.277805	1.503287
	6	-2.324306	-1.623786	-1.411566
	6	-3.806889	-0.487541	0.922429
PMe-16-2S(C_2)	8	4.877031	0.148030	-1.524507
	8	2.855366	-1.681765	2.557906
	8	-2.441631	-2.175338	-2.407247
	8	-4.826720	-0.319494	1.419226
	6	1.349120	-1.626638	-1.176892
	8	0.756010	-2.320598	-1.868738
	6	-1.041308	-1.441013	1.317220
	8	-0.377780	-1.941040	2.106284

15	1.423518	1.398478	0.254155
15	-1.677614	1.377707	-0.448975
6	0.820896	1.733035	1.944779
1	1.640601	1.567765	2.644488
1	0.463166	2.757883	2.062308
1	0.022916	1.038449	2.207370
6	2.576146	2.800024	0.025439
1	2.114143	3.757052	0.276092
1	3.452110	2.654816	0.657811
1	2.918507	2.832900	-1.008746
6	0.032572	1.963349	-0.819378
1	0.268942	1.620494	-1.829928
1	0.011196	3.058574	-0.850818
6	-2.506911	1.920110	-1.984115
1	-3.584321	1.797615	-1.872884
1	-2.292772	2.964881	-2.217993
1	-2.185782	1.296700	-2.818263
6	-2.276922	2.655894	0.713125
1	-2.015273	3.664732	0.386841
1	-3.362958	2.579694	0.775377
1	-1.882043	2.490524	1.713495

PMe-16-3S(C_1)

15	-1.651137	0.943445	0.221733
15	1.651139	0.943445	-0.221734
28	3.321594	-0.502097	0.075174
28	-3.321595	-0.502096	-0.075176
6	4.790846	0.339941	-0.530217
6	3.359534	-0.821728	1.845345
6	2.885585	-1.949382	-0.903926
6	-3.359543	-0.821719	-1.845349
6	-4.790845	0.339941	0.530226
6	-2.885582	-1.949387	0.903917
8	5.707767	0.901475	-0.928268
8	2.587597	-2.858344	-1.534987
8	3.364165	-1.001102	2.977791
8	-5.707763	0.901471	0.928286
8	-3.364176	-1.001087	-2.977795
8	-2.587596	-2.858351	1.534975
6	0.000001	0.150134	-0.000004
1	0.093773	-0.524846	0.856716
1	-0.093772	-0.524840	-0.856729
6	-1.565064	1.693546	1.883026

	1	-2.536240	2.131925	2.113920
	1	-1.374857	0.915111	2.622118
	1	-0.803988	2.466670	1.977538
	6	-1.681644	2.405789	-0.867794
	1	-1.597220	2.095249	-1.909207
	1	-2.648736	2.895638	-0.750995
	1	-0.899250	3.131606	-0.642899
	6	1.565074	1.693554	-1.883024
	1	1.374869	0.915122	-2.622120
	1	0.804000	2.466680	-1.977537
	1	2.536251	2.131932	-2.113911
	6	1.681642	2.405784	0.867801
	1	0.899248	3.131602	0.642907
	1	1.597214	2.095238	1.909212
	1	2.648734	2.895634	0.751008
	28	1.303301	-0.772083	-0.057248
	28	-1.303300	-0.772086	-0.057247
	6	2.539136	-1.606377	-1.048467
	6	1.437622	-1.342149	1.651568
	6	-2.539133	-1.606388	-1.048459
	8	3.359560	-2.127162	-1.655896
	8	1.603801	-1.657281	2.742567
	8	-3.359555	-2.127180	-1.655885
	6	-0.000001	-0.576971	-1.470947
	8	-0.000002	-0.314902	-2.612601
	6	-1.437614	-1.342144	1.651571
	8	-1.603788	-1.657268	2.742573
	15	-1.541005	1.441131	0.128844
PMe-15-1S(C_S)	15	1.541000	1.441135	0.128847
	6	1.844716	2.399903	-1.394041
	1	1.722797	3.474090	-1.242215
	1	2.865074	2.208183	-1.727149
	1	1.180164	2.068530	-2.190785
	6	2.795028	2.138321	1.256918
	1	3.790218	1.873363	0.900427
	1	2.726635	3.225348	1.327714
	1	2.672768	1.708763	2.251051
	6	-0.000004	2.188135	0.808150
	1	-0.000005	3.280499	0.728784
	1	-0.000005	1.932813	1.872642
	6	-1.844720	2.399897	-1.394046
	1	-2.865077	2.208176	-1.727155

	1	-1.722801	3.474085	-1.242221
	1	-1.180166	2.068524	-2.190788
	6	-2.795037	2.138315	1.256911
	1	-2.726647	3.225343	1.327707
	1	-3.790226	1.873355	0.900418
	1	-2.672779	1.708758	2.251045
	15	0.978597	1.703530	0.203921
	15	0.113512	-1.367760	0.030971
	28	1.985108	-0.239500	-0.115444
	28	-1.886901	0.097263	0.006264
	6	2.650271	-0.445140	-1.756566
	6	2.947527	-0.687531	1.303812
	6	-2.436273	-1.225296	-1.067683
	6	-2.809963	-0.217302	1.585998
	6	-2.463498	1.539191	-0.948832
	8	3.066119	-0.597811	-2.819499
	8	3.536770	-0.993179	2.245859
	8	-3.256635	-0.393286	2.618247
	8	-2.894599	-2.013620	-1.757432
	8	-2.816068	2.476175	-1.493903
	6	-0.615692	1.369518	1.028558
	1	-0.386249	0.854992	1.966008
PMe-15-2S(C_1)	1	-1.142850	2.295020	1.291167
	6	1.679981	3.005800	1.286038
	1	2.604607	3.387177	0.852464
	1	0.987338	3.838903	1.422973
	1	1.919301	2.582582	2.261187
	6	0.523030	2.701474	-1.256126
	1	1.429567	3.117183	-1.696463
	1	0.053760	2.071022	-2.011031
	1	-0.152609	3.522525	-1.005050
	6	-0.024759	-2.815611	-1.094404
	1	-0.021704	-2.494306	-2.135205
	1	0.873013	-3.415910	-0.933841
	1	-0.896077	-3.446457	-0.917704
	6	-0.226729	-2.222252	1.622530
	1	0.565090	-2.954766	1.797719
	1	-0.207281	-1.510498	2.447747
	1	-1.185426	-2.744721	1.627553

	28	1.130181	-0.828869	-0.076461
	28	-1.239521	-0.741048	0.063775
	6	2.561686	-1.868071	-0.036666
	6	-2.767160	-1.617786	0.205472
	8	3.524185	-2.494869	0.010261
	8	-3.785655	-2.138977	0.317100
	6	-0.156503	-1.620584	-1.279649
	8	-0.221400	-2.324601	-2.200598
	6	-0.023570	-0.909925	1.527978
	8	0.120913	-0.948020	2.677498
	15	-1.442028	1.492152	-0.077440
	15	1.581465	1.369702	0.008650
	6	-1.607604	2.150504	-1.776184
	1	-2.592286	1.890426	-2.164796
	1	-1.493034	3.236032	-1.813791
PMe-14-1S(C_1)	1	-0.871026	1.686204	-2.430591
	6	-2.739205	2.441373	0.792023
	1	-2.647402	3.516197	0.625671
	1	-3.719655	2.116529	0.443998
	1	-2.686220	2.244284	1.862238
	6	0.088891	2.315822	0.527918
	1	0.050276	2.257699	1.619501
	1	0.139210	3.373200	0.252347
	6	2.098007	2.225262	-1.522984
	1	2.198856	3.302079	-1.374773
	1	3.059274	1.826297	-1.846201
	1	1.383445	2.043262	-2.323853
	6	2.835614	1.973762	1.191667
	1	3.811209	1.567863	0.924102
	1	2.900329	3.063246	1.209501
	1	2.591695	1.616129	2.192175
	15	-1.417758	1.106237	-0.830535
	15	0.368152	-1.559084	-0.605605
	28	-0.968338	-0.465231	0.743926
	28	1.354740	0.385249	-0.297110
	6	-0.360141	0.483769	2.124995
PMe-14-2S(C_1)	6	-2.244798	-1.588066	1.268703
	6	2.873737	-0.445272	0.095589
	6	1.698702	2.041634	0.281488
	8	-0.065996	1.113408	3.042311
	8	-3.067768	-2.322163	1.590052
	8	3.881871	-0.951185	0.300439

	8	1.943320	3.110300	0.603002
	6	-2.796239	1.081705	-2.040918
	1	-3.752212	1.151373	-1.520771
	1	-2.718465	1.910648	-2.747113
	1	-2.791385	0.146823	-2.600182
	6	-1.597608	2.800994	-0.172253
	1	-1.562726	3.546459	-0.969489
	1	-2.550536	2.890330	0.349461
	1	-0.809970	3.018190	0.547635
	6	1.315609	-3.045010	-0.115950
	1	0.637864	-3.899838	-0.081834
	1	2.119198	-3.275575	-0.817477
	1	1.740438	-2.911647	0.876982
	6	-0.135791	-2.058994	-2.289992
	1	0.724935	-2.196447	-2.946350
	1	-0.665301	-3.011097	-2.219340
	1	-0.811648	-1.335392	-2.737174
	6	0.133212	1.176233	-1.761832
	1	0.388504	2.185206	-2.092616
	1	0.124652	0.528354	-2.635894
	28	0.051134	-2.193582	0.541277
	28	-0.051134	2.193582	0.541277
	6	-0.455876	-1.639443	2.161446
	6	0.277342	-3.946743	0.372063
	6	0.455876	1.639443	2.161446
	6	-0.277342	3.946743	0.372063
	8	-0.834637	-1.368502	3.214158
	8	0.425084	-5.080683	0.220294
	8	-0.425084	5.080683	0.220294
	8	0.834637	1.368502	3.214158
PMe-24-1S(C_2)	15	-1.511461	-1.728295	-0.941594
	15	-1.958306	1.309352	-0.167494
	15	1.958306	-1.309352	-0.167494
	15	1.511461	1.728295	-0.941594
	6	3.146064	-0.665837	1.063522
	1	3.369016	-1.458302	1.778016
	1	4.080741	-0.336164	0.603482
	1	2.704834	0.158849	1.621737
	6	3.017910	-2.535723	-1.023579
	1	3.967903	-2.107697	-1.351149
	1	3.219304	-3.370223	-0.351528
	1	2.492523	-2.935854	-1.891826

	6	1.973360	0.014949	-1.456968
	1	1.243818	-0.293554	-2.211872
	1	2.949990	0.045992	-1.955019
	6	1.270055	2.467769	-2.602132
	1	1.153788	3.547347	-2.499729
	1	2.109639	2.266242	-3.271372
	1	0.359365	2.080312	-3.060715
	6	3.146064	2.442004	-0.530913
	1	3.899483	2.220333	-1.290469
	1	3.035278	3.523662	-0.449442
	1	3.492969	2.077379	0.434197
	6	-3.146064	0.665837	1.063522
	1	-3.369016	1.458302	1.778016
	1	-4.080741	0.336164	0.603482
	1	-2.704834	-0.158849	1.621737
	6	-3.017910	2.535723	-1.023579
	1	-3.967903	2.107697	-1.351149
	1	-3.219304	3.370223	-0.351528
	1	-2.492523	2.935854	-1.891826
	6	-1.973360	-0.014949	-1.456968
	1	-1.243818	0.293554	-2.211872
	1	-2.949990	-0.045992	-1.955019
	6	-3.146064	-2.442004	-0.530913
	1	-3.899483	-2.220333	-1.290469
	1	-3.035278	-3.523662	-0.449442
	1	-3.492969	-2.077379	0.434197
	6	-1.270055	-2.467769	-2.602132
	1	-1.153788	-3.547347	-2.499729
	1	-2.109639	-2.266242	-3.271372
	1	-0.359365	-2.080312	-3.060715
	28	2.243486	-0.618111	0.000000
	28	-2.243486	0.618111	0.000000
	6	3.508110	-1.868278	0.000000
	6	-3.508110	1.868278	0.000000
	8	4.312192	-2.694269	0.000000
	8	-4.312192	2.694269	0.000000
PMe-24-2S(C_{2h})	15	1.088339	-1.150322	1.832139
	15	-1.088339	1.150322	1.832139
	15	1.088339	-1.150322	-1.832139
	15	-1.088339	1.150322	-1.832139
	6	-2.844415	-1.049620	0.000000
	8	-3.295665	-2.112671	0.000000

	6	2.844415	1.049620	0.000000
	8	3.295665	2.112671	0.000000
	6	0.000000	0.000000	-2.783315
	1	-0.637104	-0.603677	-3.436682
	1	0.637104	0.603677	-3.436682
	6	2.198916	-1.667259	-3.194645
	1	2.794852	-2.520238	-2.869563
	1	1.642623	-1.947450	-4.091907
	1	2.886993	-0.859057	-3.441034
	6	0.000000	-2.617977	-1.750614
	1	-0.330707	-2.918486	-2.747404
	1	0.535774	-3.450338	-1.294265
	1	-0.878761	-2.405325	-1.144519
	6	-2.198916	1.667259	-3.194645
	1	-2.794852	2.520238	-2.869563
	1	-1.642623	1.947450	-4.091907
	1	-2.886993	0.859057	-3.441034
	6	0.000000	2.617977	-1.750614
	1	0.330707	2.918486	-2.747404
	1	-0.535774	3.450338	-1.294265
	1	0.878761	2.405325	-1.144519
	6	0.000000	2.617977	1.750614
	1	-0.535774	3.450338	1.294265
	1	0.330707	2.918486	2.747404
	1	0.878761	2.405325	1.144519
	6	-2.198916	1.667259	3.194645
	1	-1.642623	1.947450	4.091907
	1	-2.794852	2.520238	2.869563
	1	-2.886993	0.859057	3.441034
	6	0.000000	0.000000	2.783315
	1	-0.637104	-0.603677	3.436682
	1	0.637104	0.603677	3.436682
	6	2.198916	-1.667259	3.194645
	1	1.642623	-1.947450	4.091907
	1	2.794852	-2.520238	2.869563
	1	2.886993	-0.859057	3.441034
	6	0.000000	-2.617977	1.750614
	1	0.535774	-3.450338	1.294265
	1	-0.330707	-2.918486	2.747404
	1	-0.878761	-2.405325	1.144519
PMe-23-1S(C_1)	28	1.037476	0.509526	-0.668368
	28	-1.312204	-0.644878	-0.547985

6	1.854740	1.460888	-1.926376
6	0.066282	-0.728143	-1.840244
6	-2.670615	-1.382454	-1.404066
8	2.421049	2.125599	-2.680414
8	-3.600810	-1.858204	-1.893540
8	0.353921	-1.303274	-2.821036
15	0.658679	2.064840	0.875833
15	-2.116273	1.228971	0.289919
15	2.246024	-1.158652	0.156504
15	-0.527441	-1.975948	1.036036
6	3.428325	-1.937627	-1.000728
1	4.233534	-1.236290	-1.221414
1	3.861356	-2.857379	-0.602085
1	2.916038	-2.159040	-1.937166
6	3.295945	-1.035445	1.656857
1	3.803877	-1.977469	1.874708
1	4.050438	-0.262242	1.509923
1	2.698911	-0.755193	2.523731
6	1.151061	-2.584514	0.578169
1	1.587498	-3.243546	1.335857
1	1.020151	-3.166588	-0.338389
6	-0.209869	-1.338329	2.725796
1	-1.154705	-1.076180	3.205018
1	0.316523	-2.055817	3.360586
1	0.388277	-0.429713	2.645490
6	-1.371289	-3.553217	1.434836
1	-0.811421	-4.162694	2.147340
1	-2.356994	-3.345748	1.852055
1	-1.518266	-4.125886	0.519191
6	-2.358124	2.560120	-0.941976
1	-3.155744	2.263724	-1.623957
1	-2.622798	3.517510	-0.485759
1	-1.452024	2.673181	-1.537129
6	-3.748046	1.250780	1.125395
1	-4.044333	2.252351	1.443757
1	-4.506119	0.860367	0.445826
1	-3.721499	0.598351	1.998707
6	-1.056931	2.053218	1.546755
1	-1.064629	1.412439	2.432154
1	-1.414379	3.043916	1.847700
6	0.817675	3.790123	0.274289
1	0.553477	4.520329	1.042058
1	1.849458	3.963602	-0.033798
1	0.189069	3.950611	-0.599937

	6	1.654633	2.229230	2.412801
	1	2.707487	2.345019	2.152748
	1	1.345350	3.094567	3.002588
	1	1.563012	1.338769	3.034597
	28	0.000576	-1.242470	-0.451210
	28	0.133396	1.243632	-0.432582
	6	0.306961	-2.735470	-1.329181
	6	-0.229219	0.109940	-1.817469
	8	0.538972	-3.741333	-1.848986
	8	-0.509118	0.271382	-2.947928
	15	1.574605	-1.084329	1.092483
	15	2.273653	1.547781	-0.188750
	15	-2.042940	-1.140015	0.425933
	15	-1.778331	1.908990	0.314658
	6	-3.350465	-1.334557	-0.842053
	1	-3.327873	-2.361751	-1.207460
	1	-4.349280	-1.121643	-0.453294
	1	-3.149594	-0.687428	-1.694684
	6	-2.676606	-2.309622	1.691334
	1	-3.725813	-2.128106	1.935477
	1	-2.577638	-3.329642	1.318941
	1	-2.088488	-2.231305	2.605521
PMe-22-1S(C_1)	6	-2.514924	0.467110	1.205890
	1	-2.063864	0.467365	2.202990
	1	-3.598939	0.562705	1.338526
	6	-2.185116	3.247903	1.506280
	1	-1.916898	4.212601	1.075233
	1	-3.246082	3.265920	1.766454
	1	-1.603784	3.121447	2.419599
	6	-3.026189	2.269774	-0.979470
	1	-4.046241	2.238226	-0.589693
	1	-2.839757	3.266059	-1.380999
	1	-2.932497	1.565710	-1.804457
	6	3.333699	0.731328	-1.438778
	1	3.325811	1.304807	-2.365731
	1	4.367609	0.619621	-1.102962
	1	2.910407	-0.250327	-1.659028
	6	3.295015	3.020008	0.209290
	1	4.331253	2.759422	0.435819
	1	3.290223	3.707445	-0.636785
	1	2.869369	3.546437	1.063308
	6	2.558879	0.481611	1.282613

	1	2.180784	1.024193	2.151773
	1	3.617777	0.266531	1.462767
	6	2.932234	-2.303688	0.899418
	1	3.677892	-2.229124	1.694056
	1	2.513280	-3.310288	0.899225
	1	3.424468	-2.158185	-0.062220
	6	1.134860	-1.394257	2.848127
	1	0.686861	-2.383760	2.944188
	1	2.002465	-1.338686	3.509918
	1	0.398946	-0.658023	3.174155
	28	0.632491	1.133634	0.087016
	28	-0.632491	-1.133634	-0.087016
	6	2.242603	1.766842	-0.171700
	6	-2.242603	-1.766842	0.171700
	8	3.283188	2.223784	-0.403898
	8	-3.283188	-2.223784	0.403898
	15	-0.418057	1.479673	1.979235
	15	0.421699	-1.261862	1.807552
	15	-0.421699	1.261862	-1.807552
	15	0.418057	-1.479673	-1.979235
	6	-2.229843	1.129689	-2.088411
	1	-2.756223	1.795338	-1.403473
	1	-2.504618	1.390484	-3.113864
	1	-2.552016	0.111012	-1.871282
	6	-0.105998	2.864354	-2.645566
PMe-22-2S(C_i)	1	-0.529055	2.883442	-3.652698
	1	-0.550148	3.675062	-2.067902
	1	0.966761	3.045968	-2.702480
	6	0.219025	0.032886	-3.020070
	1	1.176454	0.374821	-3.420110
	1	-0.460493	-0.135245	-3.859962
	6	2.235956	-1.703503	-1.964935
	1	2.489487	-2.602240	-1.400916
	1	2.654588	-1.790404	-2.970268
	1	2.687972	-0.850368	-1.457294
	6	-0.074745	-2.833982	-3.111389
	1	0.484466	-2.816405	-4.049045
	1	0.092775	-3.794763	-2.624386
	1	-1.139543	-2.757653	-3.330395
	6	0.105998	-2.864354	2.645566
	1	0.550148	-3.675062	2.067902
	1	0.529055	-2.883442	3.652698

	1	-0.966761	-3.045968	2.702480
	6	2.229843	-1.129689	2.088411
	1	2.504618	-1.390484	3.113864
	1	2.756223	-1.795338	1.403473
	1	2.552016	-0.111012	1.871282
	6	-0.219025	-0.032886	3.020070
	1	0.460493	0.135245	3.859962
	1	-1.176454	-0.374821	3.420110
	6	-2.235956	1.703503	1.964935
	1	-2.654588	1.790404	2.970268
	1	-2.489487	2.602240	1.400916
	1	-2.687972	0.850368	1.457294
	6	0.074745	2.833982	3.111389
	1	-0.092775	3.794763	2.624386
	1	-0.484466	2.816405	4.049045
	1	1.139543	2.757653	3.330395
	28	1.253103	-0.050877	0.000000
	28	-1.130647	-0.268222	0.000000
	15	1.560995	-0.008420	2.174331
	15	-1.622745	-0.019924	2.126516
	15	1.560995	-0.008420	-2.174331
	15	-1.622745	-0.019924	-2.126516
	6	-0.171208	-1.782687	0.000000
	8	0.466136	-2.761565	0.000000
	6	-0.057520	1.280438	0.000000
	8	0.040129	2.457765	0.000000
	6	-2.802362	-1.010720	-3.122939
	1	-3.823360	-0.740309	-2.854086
PMe-22-3S(C_S)	1	-2.670913	-0.857641	-4.196700
	1	-2.669570	-2.068868	-2.898594
	6	-1.908653	1.641310	-2.844374
	1	-1.760773	1.655317	-3.926853
	1	-2.930099	1.955939	-2.629158
	1	-1.240715	2.367668	-2.382555
	6	-0.042506	-0.518957	-2.971468
	1	-0.047916	-0.228872	-4.028784
	1	-0.040979	-1.613400	-2.939561
	6	1.809424	1.662390	-2.878839
	1	2.842087	1.970760	-2.716070
	1	1.600581	1.687308	-3.950719
	1	1.168321	2.382340	-2.371527
	6	2.708420	-0.989893	-3.216520

	1	2.522503	-0.850638	-4.284199
	1	3.736413	-0.701953	-2.997646
	1	2.601481	-2.047945	-2.976889
	6	-1.908653	1.641310	2.844374
	1	-2.930099	1.955939	2.629158
	1	-1.760773	1.655317	3.926853
	1	-1.240715	2.367668	2.382555
	6	-0.042506	-0.518957	2.971468
	1	-0.040979	-1.613400	2.939561
	1	-0.047916	-0.228872	4.028784
	6	2.708420	-0.989893	3.216520
	1	3.736413	-0.701953	2.997646
	1	2.522503	-0.850638	4.284199
	1	2.601481	-2.047945	2.976889
	6	1.809424	1.662390	2.878839
	1	1.600581	1.687308	3.950719
	1	2.842087	1.970760	2.716070
	1	1.168321	2.382340	2.371527
	6	-2.802362	-1.010720	3.122939
	1	-2.670913	-0.857641	4.196700
	1	-3.823360	-0.740309	2.854086
	1	-2.669570	-2.068868	2.898594

Table S35. Theoretical cartesian coordinates (in Å) for the singlet and triplet structures at BP86/DZP level.

Standard orientation:

Structures	**Atomic Number**	**Coordinates (Angstroms)**		
		X	**Y**	**Z**
	7	1.197994	0.086470	0.000000
	6	2.520105	0.790371	0.000000
	1	2.338776	1.878246	0.000000
	1	3.091700	0.522434	0.903528
	1	3.091700	0.522434	-0.903528
$[MeN(PF_2)_2]Ni_2(CO)_6$	15	1.223816	-1.639966	0.000000
S-PF-16-1S(C_S)	15	-0.214529	1.051311	0.000000
	9	2.284599	-1.871173	1.199345
	9	2.284599	-1.871173	-1.199345
	9	-1.066446	0.382842	-1.198258
	9	-1.066446	0.382842	1.198258
	28	-0.134160	3.225258	0.000000

	28	-0.478452	-2.976292	0.000000
	6	-1.464815	-2.720887	-1.504056
	6	-1.464815	-2.720887	1.504056
	6	0.246264	-4.639110	0.000000
	6	0.689726	3.804818	1.508065
	6	-1.875113	3.745233	0.000000
	6	0.689726	3.804818	-1.508065
	8	-2.109706	-2.599360	-2.467641
	8	-2.109706	-2.599360	2.467641
	8	0.683742	-5.720496	0.000000
	8	-2.982473	4.108848	0.000000
	8	1.204850	4.201072	2.477346
	8	1.204850	4.201072	-2.477346
	7	0.005399	0.003172	0.143362
	6	-0.009822	1.471509	0.423761
	1	0.798826	1.966287	-0.140280
	1	-0.975837	1.885558	0.090385
	1	0.108140	1.678007	1.502054
	15	1.544250	-0.752378	0.320601
	15	-1.505384	-0.753274	-0.181026
	9	-1.358475	-2.106134	0.678240
	9	1.444252	-1.395812	1.797917
	9	-1.241795	-1.424805	-1.621203
	9	1.272339	-2.103069	-0.502412
$[MeN(PF_2)_2]Ni_2(CO)_6$	28	-3.391950	0.315309	0.015005
S-PF-16-2S(*C*$_1$)	28	3.385964	0.317115	-0.107265
	6	-3.474540	1.108843	1.643235
	8	-3.553495	1.619446	2.689965
	6	-4.660388	-0.977198	-0.122720
	6	-3.557061	1.504460	-1.343614
	6	4.677444	-0.959164	-0.152480
	6	3.708838	1.501682	1.226429
	6	3.234300	1.124049	-1.723674
	8	-5.493015	-1.788646	-0.206863
	8	-3.690214	2.267609	-2.216591
	8	3.164002	1.643338	-2.766582
	8	3.933521	2.264583	2.080744
	8	5.521225	-1.762809	-0.186239

	7	0.013191	2.057324	0.068898
	6	-0.050031	3.554209	0.185205
	1	0.887764	3.914641	0.633412
	1	-0.165188	4.012539	-0.810903
	1	-0.890651	3.844734	0.833449
	15	-1.346203	1.201215	-0.560580
	15	1.485671	1.265051	0.433326
	9	-1.124473	1.354826	-2.157301
	9	2.511946	2.381109	-0.134809
	9	-2.407557	2.410355	-0.414222
	9	1.664108	1.675168	1.988078
	28	-2.156819	-0.667272	0.197989
$[MeN(PF_2)_2]Ni_2(CO)_6$	28	2.079573	-0.740389	-0.147376
S-PF-16-3S(*C*$_1$)	6	-1.763612	-0.796023	1.965048
	6	3.890446	-0.686907	-0.018652
	6	-3.950206	-0.473882	-0.008331
	6	1.629585	-1.046739	-1.879152
	8	-1.564977	-0.879448	3.111410
	8	5.054133	-0.687667	0.053030
	8	-5.106495	-0.381567	-0.126669
	8	1.406982	-1.264157	-3.002991
	6	1.461874	-2.003199	1.003533
	8	1.130709	-2.844073	1.740520
	6	-1.617178	-2.102944	-0.777535
	8	-1.327215	-3.044696	-1.400680

	7	0.001987	2.286485	0.013119
	6	0.013640	3.776833	-0.008679
	1	-0.973491	4.147046	0.311512
	1	0.770288	4.144432	0.703927
	1	0.239699	4.148401	-1.021672
	15	1.421624	1.350664	0.097718
	15	-1.419077	1.355986	-0.090339
$[MeN(PF_2)_2]Ni_2(CO)_5$	9	2.126732	1.989569	1.405768
S-PF-15-1S(*C*$_1$)	9	2.340616	2.147579	-0.968479
	9	-2.115081	2.001432	-1.400077
	9	-2.347792	2.147925	0.971780
	28	1.333856	-0.806964	-0.083673
	28	-1.335756	-0.803176	0.082352
	6	2.018821	-1.153208	-1.731646
	6	2.340462	-1.397487	1.308069
	6	-0.003366	-2.205084	-0.005479

	6	-2.019642	-1.156005	1.729717
	6	-2.345640	-1.383377	-1.311016
	8	3.025545	-1.770545	2.174567
	8	2.502649	-1.380556	-2.767963
	8	-0.005364	-3.389528	-0.009490
	8	-3.032749	-1.750791	-2.178346
	8	-2.502748	-1.387289	2.765479
$[MeN(PF_2)_2]Ni_2(CO)_5$ **S-PF-15-2S(*C*$_1$)**	7	-0.109479	2.203948	-0.018101
	6	-0.169860	3.695292	0.028270
	1	-1.024777	4.040309	-0.575664
	1	-0.279290	4.047606	1.067117
	1	0.752946	4.106864	-0.411005
	15	-1.531783	1.262015	-0.075008
	15	1.377449	1.369098	0.098347
	9	-2.409659	1.987503	1.073560
	9	2.254330	2.220741	-0.961789
	9	-2.297362	1.966766	-1.313472
	9	2.014177	2.071230	1.410470
	28	-1.273909	-0.895002	0.001970
	28	1.352062	-0.803057	-0.061362
	6	-1.378090	-1.368195	1.760677
	6	2.751815	-1.325847	-1.072326
	6	-2.629722	-1.748983	-0.831785
	8	-1.521470	-1.687455	2.873439
	8	3.689874	-1.643980	-1.686724
	8	-3.542454	-2.274079	-1.331828
	6	1.627179	-1.530732	1.590270
	8	1.885137	-2.018277	2.617833
	6	0.019941	-1.209560	-1.422937
	8	-0.003177	-1.480139	-2.576820
$[MeN(PF_2)_2]Ni_2(CO)_5$ **S-PF-15-1T(*C*$_1$)**	7	-0.972874	2.031671	-0.007871
	6	-1.518443	3.422443	0.035090
	1	-0.751239	4.124964	-0.327076
	1	-2.389171	3.483275	-0.637747
	1	-1.819381	3.690257	1.061329
	15	-2.000654	0.670351	-0.146801
	15	0.684458	1.722874	0.245142
	9	-2.849918	1.077110	-1.458585
	9	-3.152661	1.076222	0.912827

	9	0.934812	2.405938	1.688828
	9	1.331790	2.934470	-0.604491
	28	-0.940985	-1.194612	0.018779
	28	1.616465	-0.277787	-0.064674
	6	-0.615581	-1.423879	1.797902
	6	-1.864467	-2.634072	-0.573311
	6	0.337913	-1.010588	-1.429646
	6	3.281178	0.391114	-0.514898
	6	2.196381	-1.885043	0.632719
	8	-2.445777	-3.560106	-0.980424
	8	-0.535320	-1.606123	2.951122
	8	0.477849	-1.203005	-2.597048
	8	2.621896	-2.881892	1.066817
	8	4.296517	0.651764	-1.036194
$[MeN(PF_2)_2]Ni_2(CO)_4$ **S-PF-14-1S(C_1)**	7	1.108474	-1.889620	-0.174628
	15	1.922365	-0.428562	0.122109
	15	-0.581658	-1.687963	-0.352435
	9	2.675436	-0.730520	1.519006
	9	3.222665	-0.636613	-0.813098
	9	-1.080317	-3.002438	0.450361
	9	-0.817582	-2.315140	-1.823936
	28	0.753464	1.368256	-0.125490
	28	-1.443273	0.230733	0.185949
	6	1.790059	2.800384	-0.319396
	6	-1.506812	0.270927	1.998122
	6	-3.086640	0.241085	-0.571931
	8	2.489724	3.727509	-0.444625
	8	-1.584247	0.312821	3.161768
	8	-4.156918	0.225691	-1.033521
	6	-0.963953	2.041339	-0.437153
	8	-1.547976	3.012428	-0.789353
	6	1.771358	-3.221515	-0.232988
	1	2.812823	-3.090443	-0.568598
	1	1.754419	-3.709947	0.755404
	1	1.246940	-3.854615	-0.967421
$[MeN(PF_2)_2]Ni_2(CO)_4$ **S-PF-14-2S(C_S)**	7	0.014804	2.201838	0.000000
	6	-0.021240	3.692208	0.000000
	1	0.504946	4.067016	0.893085
	1	0.504946	4.067016	-0.893085

	1	-1.061921	4.056215	0.000000
	15	0.006026	1.297894	-1.449536
	15	0.006026	1.297894	1.449536
	9	1.201094	2.028937	-2.255950
	9	1.201094	2.028937	2.255950
	9	-1.196611	2.028823	-2.244184
	9	-1.196611	2.028823	2.244184
	28	0.001018	-0.882183	-1.195602
	28	0.001018	-0.882183	1.195602
	6	-0.004341	-1.878382	-2.675859
	6	-0.004341	-1.878382	2.675859
	8	-0.008353	-2.504473	-3.662083
	8	-0.008353	-2.504473	3.662083
	6	-1.429158	-1.475452	0.000000
	8	-2.489744	-1.987834	0.000000
	6	1.427119	-1.486248	0.000000
	8	2.484162	-2.005695	0.000000
	7	-0.726006	1.972467	-0.178675
	6	-1.536402	3.187844	-0.119173
	1	-2.009936	3.313311	0.874361
	1	-0.919625	4.082971	-0.324036
	1	-2.337497	3.144597	-0.880240
	15	0.833922	1.709224	-0.013923
	28	-1.353936	0.066318	0.003639
	28	1.298655	-0.457023	-0.045021
	9	1.651063	2.609363	-1.096284
	9	1.428700	2.507256	1.279369
	6	-2.196536	0.070027	1.612823
	6	-2.278608	-0.135215	-1.548613
	6	2.046828	-0.767849	-1.665480
	6	2.270253	-0.751279	1.451591
	8	2.918251	-0.940030	2.401303
	8	2.554213	-0.962024	-2.696235
	8	-2.807511	0.076115	2.604995
	8	-2.933118	-0.241051	-2.506427
	15	-0.337337	-1.805701	0.092879
	9	-0.656408	-2.917658	-1.027848
	9	-0.561101	-2.759685	1.371318

$[MeN(PF_2)_2]Ni_2(CO)_4$
S-PF-14-3S(*C*$_1$)

	7	0.799359	1.771773	-0.028782
	6	1.428587	3.107067	-0.006562
	1	2.517137	3.005358	-0.143182
	1	1.025203	3.752565	-0.811239
	1	1.237481	3.612806	0.960882
	15	-0.886452	1.678299	-0.018422
	28	1.802467	0.158129	-0.022846
	28	-1.757241	-0.341575	-0.010733
	9	-1.299222	2.693449	1.182786
	9	-1.309826	2.686487	-1.221281
$[MeN(PF_2)_2]Ni_2(CO)_4$	6	2.771007	-0.422179	-1.455538
S-PF-14-1T(*C*$_1$)	6	2.826461	-0.314320	1.409556
	6	-2.601388	-0.781883	1.520873
	6	-2.513682	-0.823919	-1.576141
	8	-2.987591	-1.163898	-2.587731
	8	-3.131408	-1.096312	2.512666
	8	3.371360	-0.854463	-2.355789
	8	3.460101	-0.679988	2.316576
	15	0.140108	-1.405878	0.061744
	9	0.321302	-2.384753	1.346851
	9	0.330845	-2.545659	-1.080968

	7	2.054236	-0.018748	0.000000
	6	3.547639	0.020122	0.000000
	1	3.922273	-0.507261	0.892155
	1	3.922273	-0.507261	-0.892155
	1	3.909538	1.061250	0.000000
	15	1.169377	-0.007494	-1.464573
	15	1.169377	-0.007494	1.464573
	9	1.909837	1.182773	-2.264745
	9	1.898408	-1.196434	-2.277589
	9	1.909837	1.182773	2.264745
$[MeN(PF_2)_2]Ni_2(CO)_4$	9	1.898408	-1.196434	2.277589
S-PF-14-2T(*C*$_S$/*C*$_1$)	28	-0.959210	0.001426	-1.153881
	28	-0.959210	0.001426	1.153881
	6	-1.269642	1.574028	0.000000
	6	-1.771143	0.006279	-2.755686
	6	-1.771143	0.006279	2.755686
	6	-1.288894	-1.567006	0.000000
	8	-1.498895	2.737029	0.000000
	8	-2.280151	0.009890	-3.807905
	8	-2.280151	0.009890	3.807905
	8	-1.531877	-2.727159	0.000000

	7	2.498296	0.000000	-0.849831
	6	3.777980	0.000000	-1.639109
	1	4.366463	0.891824	-1.373461
	1	4.366463	-0.891824	-1.373461
	1	3.561621	0.000000	-2.719124
	15	1.817529	-1.514935	-0.439133
	15	1.817529	1.514935	-0.439133
	9	3.117617	-2.205110	0.238204
	9	1.995742	-2.244591	-1.874130
	9	1.995742	2.244591	-1.874130
	9	3.117617	2.205110	0.238204
	28	0.000000	-2.048931	0.585553
	28	0.000000	2.048931	0.585553
	15	-1.817529	-1.514935	-0.439133
	15	-1.817529	1.514935	-0.439133
$[MeN(PF_2)_2]_2Ni_2(CO)_4$	9	-3.117617	-2.205110	0.238204
S-PF-24-1S(C_{2v})	9	-1.995742	-2.244591	-1.874130
	9	-1.995742	2.244591	-1.874130
	9	-3.117617	2.205110	0.238204
	6	0.000000	-1.673177	2.352696
	6	0.000000	-3.847683	0.412573
	6	0.000000	3.847683	0.412573
	6	0.000000	1.673177	2.352696
	8	0.000000	-5.012436	0.345284
	8	0.000000	-1.570602	3.515100
	8	0.000000	5.012436	0.345284
	8	0.000000	1.570602	3.515100
	7	-2.498296	0.000000	-0.849831
	6	-3.777980	0.000000	-1.639109
	1	-4.366463	-0.891824	-1.373461
	1	-4.366463	0.891824	-1.373461
	1	-3.561621	0.000000	-2.719124

	7	-0.002170	2.733593	-0.053416
	6	-0.061357	4.229010	-0.140519
	1	-0.359687	4.646769	0.835188
$[MeN(PF_2)_2]_2Ni_2(CO)_4$	1	0.939057	4.610259	-0.391376
S-PF-24-2S(C_S)	1	-0.779503	4.541025	-0.915371
	15	1.400047	1.866661	-0.517124
	15	-1.376190	1.866388	0.507530
	9	2.496783	3.017872	-0.212367

	9	1.406850	2.075399	-2.123031
	9	-2.465221	3.034475	0.254151
	9	-1.277024	2.084326	2.108979
	28	2.003103	0.000013	0.385569
	28	-2.034971	-0.000017	-0.352512
	15	1.400076	-1.866643	-0.517125
	15	-1.376153	-1.866403	0.507543
	9	2.496829	-3.017840	-0.212371
	9	1.406883	-2.075378	-2.123032
	9	-2.465169	-3.034510	0.254196
	9	-1.276955	-2.084321	2.108993
	6	3.802032	0.000028	0.195435
	6	-3.823651	-0.000033	-0.085516
	8	4.965334	0.000037	0.105097
	8	-4.981802	-0.000045	0.057270
	7	-0.002129	-2.733593	-0.053419
	6	-0.061299	-4.229010	-0.140532
	1	0.939113	-4.610244	-0.391422
	1	-0.359594	-4.646782	0.835179
	1	-0.779462	-4.541028	-0.915366
	6	1.562726	0.000014	2.135820
	8	1.372325	0.000018	3.287445
	6	-1.644846	-0.000019	-2.113816
	8	-1.473684	-0.000021	-3.268792

$[MeN(PF_2)_2]_2Ni_2(CO)_4$ **S-PF-24-1T(*Cs*)**	7	-0.084766	-0.495999	2.849577
	6	-0.192937	-1.002802	4.255243
	1	0.323344	-0.306759	4.936720
	1	-1.255676	-1.041678	4.538127
	1	0.252126	-2.007239	4.338006
	15	-1.444057	-0.479134	1.802332
	15	1.425143	0.013025	2.237331
	9	-2.581697	-0.126403	2.903159
	9	-1.794543	-2.057618	1.729954
	9	2.367567	-0.942448	3.151867
	9	1.704769	1.374764	3.065653
	28	-1.602781	0.714354	0.000000
	28	1.701374	-0.035221	0.000000
	15	-1.444057	-0.479134	-1.802332
	15	1.425143	0.013025	-2.237331
	9	-2.581697	-0.126403	-2.903159
	9	-1.794543	-2.057618	-1.729954

	9	2.367567	-0.942448	-3.151867
	9	1.704769	1.374764	-3.065653
	6	-3.356633	1.211248	0.000000
	6	2.755782	1.501593	0.000000
	8	-4.457008	1.597072	0.000000
	8	3.588253	2.327103	0.000000
	7	-0.084766	-0.495999	-2.849577
	6	-0.192937	-1.002802	-4.255243
	1	-1.255676	-1.041678	-4.538127
	1	0.323344	-0.306759	-4.936720
	1	0.252126	-2.007239	-4.338006
	6	-0.656652	2.259724	0.000000
	8	-0.194462	3.332864	0.000000
	6	1.618111	-1.887626	0.000000
	8	1.810192	-3.047347	0.000000

$[MeN(PF_2)_2]_2Ni_2(CO)_4$
S-PF-24-2T(*C*$_2$)

7	0.080911	2.540297	-1.048647
6	0.080911	3.781907	-1.880065
1	-0.664440	4.486582	-1.476966
1	1.073227	4.255948	-1.817336
1	-0.157424	3.545612	-2.929940
15	1.507797	1.641956	-0.788109
15	-1.367680	1.943805	-0.375666
9	2.532812	2.844880	-0.450329
9	2.009925	1.445171	-2.316027
9	-2.356408	2.169297	-1.636680
9	-1.880120	3.239554	0.442078
28	1.499769	-0.004900	0.602762
28	-1.499769	0.004900	0.602762
15	1.367680	-1.943805	-0.375666
15	-1.507797	-1.641956	-0.788109
9	1.880120	-3.239554	0.442078
9	2.356408	-2.169297	-1.636680
9	-2.009925	-1.445171	-2.316027
9	-2.532812	-2.844880	-0.450329
6	0.552996	0.567639	2.210566
6	3.133226	-0.032257	1.392610
6	-3.133226	0.032257	1.392610
6	-0.552996	-0.567639	2.210566
8	4.152689	-0.020169	1.958432
8	0.574278	1.511898	2.973322
8	-4.152689	0.020169	1.958432
8	-0.574278	-1.511898	2.973322

	7	-0.080911	-2.540297	-1.048647
	6	-0.080911	-3.781907	-1.880065
	1	0.664440	-4.486582	-1.476966
	1	-1.073227	-4.255948	-1.817336
	1	0.157424	-3.545612	-2.929940

	7	2.507033	0.224907	-0.995313
	6	3.726075	0.335124	-1.847504
	1	4.206372	1.310183	-1.665854
	1	4.435867	-0.459066	-1.564221
	1	3.465749	0.239447	-2.914572
	15	1.925463	-1.287166	-0.458278
	15	1.562084	1.587658	-0.593229
	9	3.281694	-1.909692	0.169310
	9	2.008875	-2.132128	-1.837276
	9	1.374103	2.257898	-2.056583
	9	2.728919	2.606477	-0.122640
	28	0.126434	-1.293772	0.740229
	28	-0.120022	1.298978	0.736415
	15	-1.599074	-1.588703	-0.528103
$[MeN(PF_2)_2]_2Ni_2(CO)_3$	15	-1.959626	1.267997	-0.395826
S-PF-23-1S(*C*$_1$)	9	-2.748538	-2.598216	0.000324
	9	-1.455404	-2.290800	-1.981101
	9	-2.093337	2.130232	-1.760001
	9	-3.292632	1.881541	0.287195
	6	0.159619	-2.719795	1.835434
	6	-0.216402	2.738922	1.808895
	6	0.218067	0.027559	2.151689
	8	0.189787	-3.670606	2.510626
	8	-0.279153	3.699524	2.467770
	8	0.412564	0.045361	3.321121
	7	-2.553606	-0.236395	-0.934618
	6	-3.788349	-0.350978	-1.761896
	1	-4.276572	-1.316217	-1.550528
	1	-4.483937	0.457370	-1.483459
	1	-3.546496	-0.280888	-2.835250

$[MeN(PF_2)_2]_2Ni_2(CO)_3$	7	0.384875	-0.340536	2.866507
S-PF-23-2S(*C*$_S$)	6	0.423073	-0.614194	4.325760

	1	-0.485991	-1.160866	4.622500
	1	1.302063	-1.245205	4.536908
	1	0.500847	0.323212	4.903025
	15	1.719786	-0.324419	1.814239
	15	-0.957859	0.273077	1.996616
	9	2.344485	-1.799271	2.044945
	9	2.835570	0.436145	2.703537
	9	-1.072572	1.824065	2.441121
	9	-2.097210	-0.245666	3.035934
	28	1.016699	0.539198	0.000000
	28	-1.551089	-0.351960	0.000000
	15	1.719786	-0.324419	-1.814239
	15	-0.957859	0.273077	-1.996616
	9	2.344485	-1.799271	-2.044945
	9	2.835570	0.436145	-2.703537
	9	-1.072572	1.824065	-2.441121
	9	-2.097210	-0.245666	-3.035934
	6	-3.248562	0.258032	0.000000
	8	-4.356977	0.619146	0.000000
	7	0.384875	-0.340536	-2.866507
	6	0.423073	-0.614194	-4.325760
	1	1.302063	-1.245205	-4.536908
	1	-0.485991	-1.160866	-4.622500
	1	0.500847	0.323212	-4.903025
	6	-1.429413	-2.165131	0.000000
	8	-1.396614	-3.331132	0.000000
	6	1.131284	2.326648	0.000000
	8	1.266264	3.488102	0.000000

$[MeN(PF_2)_2]_2Ni_2(CO)_3$
S-PF-23-1T(C_S)

7	0.088214	-0.767696	2.734170
6	0.129999	-1.437598	4.067028
1	1.045177	-1.125374	4.595385
1	-0.740166	-1.115419	4.661701
1	0.118108	-2.534017	3.951811
15	-1.386123	-0.380108	1.981537
15	1.502997	-0.468073	1.819437
9	-2.158064	0.377356	3.182266
9	-2.192986	-1.770053	2.156845
9	2.170242	-1.943203	1.832222
9	2.450950	0.132495	2.982264
28	-1.423723	0.516548	0.000000
28	1.330648	0.654262	0.000000

	15	-1.386123	-0.380108	-1.981537
	15	1.502997	-0.468073	-1.819437
	9	-2.158064	0.377356	-3.182266
	9	-2.192986	-1.770053	-2.156845
	9	2.170242	-1.943203	-1.832222
	9	2.450950	0.132495	-2.982264
	6	-3.182365	1.048287	0.000000
	6	2.772166	1.753552	0.000000
	8	-4.179715	1.665920	0.000000
	8	3.603859	2.574041	0.000000
	7	0.088214	-0.767696	-2.734170
	6	0.129999	-1.437598	-4.067028
	1	-0.740166	-1.115419	-4.661701
	1	1.045177	-1.125374	-4.595385
	1	0.118108	-2.534017	-3.951811
	6	-0.082172	1.974112	0.000000
	8	-0.230355	3.162148	0.000000
	7	0.328738	-0.139460	2.981001
	6	0.431012	-0.201495	4.470432
	1	-0.527256	-0.550026	4.885688
	1	1.212868	-0.929457	4.742184
	1	0.681193	0.788599	4.886880
	15	1.736710	-0.177464	2.001039
	15	-1.169082	0.191407	2.209022
	9	2.438701	-1.521995	2.557800
	9	2.684907	0.850111	2.818064
	9	-1.527358	1.668258	2.772771
	9	-2.163484	-0.593603	3.219146
$[MeN(PF_2)_2]_2Ni_2(CO)_3$	28	1.065309	0.172412	0.000000
S-PF-23-2T(*C*$_S$)	28	-1.454588	-0.173913	0.000000
	15	1.736710	-0.177464	-2.001039
	15	-1.169082	0.191407	-2.209022
	9	2.438701	-1.521995	-2.557800
	9	2.684907	0.850111	-2.818064
	9	-1.527358	1.668258	-2.772771
	9	-2.163484	-0.593603	-3.219146
	6	-3.270948	-0.387446	0.000000
	8	-4.392960	-0.722964	0.000000
	7	0.328738	-0.139460	-2.981001
	6	0.431012	-0.201495	-4.470432
	1	1.212868	-0.929457	-4.742184
	1	-0.527256	-0.550026	-4.885688

	1	0.681193	0.788599	-4.886880
	6	-0.015665	-1.495935	0.000000
	8	0.128804	-2.680738	0.000000
	6	0.747147	1.952851	0.000000
	8	0.615394	3.117351	0.000000
	7	0.371405	-0.662940	2.670385
	6	0.523606	-1.402811	3.956530
	1	1.228723	-0.856950	4.604751
	1	-0.452149	-1.445687	4.466288
	1	0.897167	-2.424991	3.779096
	15	-1.099184	-0.683996	1.795424
	15	1.693641	0.136215	1.937128
	9	-2.133779	-0.416862	3.012901
	9	-1.370619	-2.279594	1.719903
	9	2.853428	-0.953245	2.246250
	9	2.137647	1.161887	3.107795
	28	-1.346449	0.517520	0.000000
	28	1.128233	0.802568	0.000000
$[MeN(PF_2)_2]_2Ni_2(CO)_2$	15	-1.099184	-0.683996	-1.795424
S-PF-22-1S(*C*$_S$)	15	1.693641	0.136215	-1.937128
	9	-2.133779	-0.416862	-3.012901
	9	-1.370619	-2.279594	-1.719903
	9	2.853428	-0.953245	-2.246250
	9	2.137647	1.161887	-3.107795
	6	-2.976452	1.251215	0.000000
	6	-0.237598	2.084311	0.000000
	8	-4.051543	1.706108	0.000000
	8	-0.202207	3.269968	0.000000
	7	0.371405	-0.662940	-2.670385
	6	0.523606	-1.402811	-3.956530
	1	-0.452149	-1.445687	-4.466288
	1	1.228723	-0.856950	-4.604751
	1	0.897167	-2.424991	-3.779096
	7	0.017443	0.024514	2.933786
	6	0.020438	0.047976	4.430143
	1	0.914981	0.584927	4.783611
$[MeN(PF_2)_2]_2Ni_2(CO)_2$	1	-0.868742	0.590791	4.788888
S-PF-22-2S(*C*$_S$)	1	0.021901	-0.977945	4.833798
	15	-1.495190	-0.103921	2.113716
	15	1.529954	0.065720	2.108069

	9	-2.322047	1.040816	2.906277
	9	-2.133999	-1.358936	2.917991
	9	2.343638	-1.010494	3.004611
	9	2.169662	1.387866	2.800341
	28	-1.082136	0.134534	0.000000
	28	1.301103	-0.325690	0.000000
	15	-1.495190	-0.103921	-2.113716
	15	1.529954	0.065720	-2.108069
	9	-2.322047	1.040816	-2.906277
	9	-2.133999	-1.358936	-2.917991
	9	2.343638	-1.010494	-3.004611
	9	2.169662	1.387866	-2.800341
	7	0.017443	0.024514	-2.933786
	6	0.020438	0.047976	-4.430143
	1	-0.868742	0.590791	-4.788888
	1	0.914981	0.584927	-4.783611
	1	0.021901	-0.977945	-4.833798
	6	-0.671245	1.886026	0.000000
	8	-0.370296	3.015752	0.000000
	6	-0.077160	-1.559872	0.000000
	8	-0.172193	-2.745694	0.000000
	7	1.992156	-1.439564	-0.478573
	6	3.178547	-2.309324	-0.755451
	1	3.552071	-2.755887	0.180183
	1	2.886585	-3.102198	-1.462809
	1	3.973446	-1.705998	-1.221958
	15	2.178114	0.239357	-0.369844
	15	0.431919	-2.155179	-0.282076
	9	3.463564	0.352990	0.596137
	9	2.982155	0.565354	-1.732661
	9	0.862587	-3.403088	0.650868
	9	0.363775	-3.013637	-1.652499
$[MeN(PF_2)_2]_2Ni_2(CO)_2$	7	-0.983718	1.828939	-1.214191
S-PF-22-1T(C_1)	15	-1.872726	0.426080	-1.251537
	28	0.447214	1.519841	0.025686
	28	-1.203041	-0.934596	0.334985
	6	-1.347404	3.036609	-1.967976
	1	-1.494896	2.801520	-3.041087
	1	-2.288681	3.479758	-1.587769
	1	-0.540715	3.782136	-1.880417
	9	-1.788311	-0.063575	-2.802092
	9	-3.431982	0.884850	-1.324782
	6	1.165607	3.067407	0.672576
	6	-2.549031	-1.827143	1.126558

	8	1.570524	4.004051	1.239387
	8	-3.412924	-2.370119	1.695551
	15	-0.397675	0.450063	1.780167
	9	-1.397949	1.304282	2.725589
	9	0.610015	-0.059773	2.948333
	7	0.064418	-0.113899	2.944709
	6	0.125577	-0.181909	4.430169
	1	-0.897625	-0.120216	4.833617
	1	0.562854	-1.147781	4.733386
	1	0.735343	0.643428	4.834398
	15	1.385254	-0.553640	1.935735
	15	-1.261038	0.470932	2.056971
	9	1.480258	-2.146866	2.209115
	9	2.589962	-0.151831	2.950053
	9	-1.354168	2.024880	2.497117
	9	-2.467635	-0.045421	3.007342
	28	1.265855	0.372430	0.000000
	28	-1.136256	-0.178203	0.000000
$[MeN(PF_2)_2]_2Ni_2(CO)_2$	15	1.385254	-0.553640	-1.935735
S-PF-22-2T(*C_{2v}* /*C_S*)	15	-1.261038	0.470932	-2.056971
	9	1.480258	-2.146866	-2.209115
	9	2.589962	-0.151831	-2.950053
	9	-1.354168	2.024880	-2.497117
	9	-2.467635	-0.045421	-3.007342
	7	0.064418	-0.113899	-2.944709
	6	0.125577	-0.181909	-4.430169
	1	0.562854	-1.147781	-4.733386
	1	-0.897625	-0.120216	-4.833617
	1	0.735343	0.643428	-4.834398
	6	-2.094091	-1.695369	0.000000
	8	-2.711042	-2.689252	0.000000
	6	1.339312	2.152896	0.000000
	8	1.397542	3.323081	0.000000
	7	0.064418	-0.113899	2.944709
	6	0.125577	-0.181909	4.430169
$[MeN(PF_2)_2]_2Ni_2(CO)_2$	1	-0.897625	-0.120216	4.833617
S-PF-22-3T(*C_S*)	1	0.562854	-1.147781	4.733386
	1	0.735343	0.643428	4.834398
	15	1.385254	-0.553640	1.935735
	15	-1.261038	0.470932	2.056971

	9	1.480258	-2.146866	2.209115
	9	2.589962	-0.151831	2.950053
	9	-1.354168	2.024880	2.497117
	9	-2.467635	-0.045421	3.007342
	28	1.265855	0.372430	0.000000
	28	-1.136256	-0.178203	0.000000
	15	1.385254	-0.553640	-1.935735
	15	-1.261038	0.470932	-2.056971
	9	1.480258	-2.146866	-2.209115
	9	2.589962	-0.151831	-2.950053
	9	-1.354168	2.024880	-2.497117
	9	-2.467635	-0.045421	-3.007342
	7	0.064418	-0.113899	-2.944709
	6	0.125577	-0.181909	-4.430169
	1	0.562854	-1.147781	-4.733386
	1	-0.897625	-0.120216	-4.833617
	1	0.735343	0.643428	-4.834398
	6	-2.094091	-1.695369	0.000000
	8	-2.711042	-2.689252	0.000000
	6	1.339312	2.152896	0.000000
	8	1.397542	3.323081	0.000000

$[(Me_2P)_2CH_2]Ni_2(CO)_6$ **S-PMe-16-1S(*C*$_1$)**	15	1.638145	1.249417	0.019928
	15	-1.252272	-0.336403	0.301323
	28	-3.436489	0.024257	-0.122827
	6	-4.311831	-1.426762	0.490440
	6	-3.583413	0.201332	-1.909932
	6	-3.878100	1.525012	0.768396
	8	-4.885744	-2.368061	0.887319
	8	-4.162953	2.503686	1.348313
	8	-3.682539	0.315599	-3.072293
	28	3.146311	-0.435241	-0.075593
	6	2.972404	-1.208376	-1.695616
	6	4.733636	0.407244	0.081821
	6	2.912682	-1.570793	1.303139
	8	2.882263	-1.709827	-2.750397
	8	5.772997	0.936409	0.189052
	8	2.804505	-2.313281	2.204013
	6	-0.540902	-1.883614	-0.409689
	1	0.544256	-1.964304	-0.222704
	1	-1.059347	-2.746831	0.043309
	1	-0.729850	-1.904932	-1.496923
	6	-0.802253	-0.461512	2.089839

	1	-1.403936	-1.272357	2.536580
	1	0.267978	-0.688260	2.241343
	1	-1.066021	0.477041	2.607365
	6	-0.175211	1.019532	-0.398839
	1	-0.695996	1.973424	-0.182427
	1	-0.229788	0.884788	-1.497399
	6	2.039493	2.615958	-1.167351
	1	1.311673	3.445818	-1.100829
	1	3.049434	3.000782	-0.941587
	1	2.048008	2.221593	-2.198105
	6	1.583649	2.177569	1.621357
	1	2.597066	2.561533	1.833120
	1	0.876889	3.026840	1.577610
	1	1.297363	1.507480	2.448214
	15	-1.676732	-0.964779	-0.234388
	15	1.676733	-0.964790	0.234369
	28	3.368751	0.494987	-0.069678
	28	-3.368746	0.494995	0.069689
	6	4.862256	-0.379315	0.428093
	6	3.368741	0.914736	-1.822114
	6	3.026852	1.917618	0.984923
	6	-3.368742	0.914704	1.822136
	6	-4.862250	-0.379311	-0.428086
	6	-3.026857	1.917634	-0.984902
	8	5.834664	-0.948428	0.751323
	8	2.817401	2.844408	1.670000
	8	3.376404	1.186096	-2.962263
	8	-5.834655	-0.948429	-0.751316
	8	-3.376417	1.186029	2.962293
	8	-2.817411	2.844425	-1.669979
	6	0.000002	-0.164090	-0.000003
	1	0.106737	0.514721	-0.868781
	1	-0.106728	0.514708	0.868786
	6	-1.598428	-1.713367	-1.924574
	1	-2.568419	-2.198857	-2.130856
	1	-1.460200	-0.910545	-2.669578
	1	-0.791958	-2.458041	-2.035613
	6	-1.741701	-2.448526	0.869196
	1	-1.665252	-2.129317	1.922773
	1	-2.730076	-2.922286	0.734397
	1	-0.957483	-3.194486	0.648257
	6	1.598427	-1.713407	1.924541

$[(Me_2P)_2CH_2]Ni_2(CO)_6$
S-PMe-16-2S(C_2)

	1	1.460226	-0.910594	2.669560
	1	0.791939	-2.458064	2.035576
	1	2.568407	-2.198925	2.130805
	6	1.741695	-2.448514	-0.869245
	1	0.957484	-3.194483	-0.648313
	1	1.665231	-2.129284	-1.922814
	1	2.730075	-2.922272	-0.734470
	28	2.518645	-0.564929	-0.134523
	28	-2.352854	-0.687632	0.139592
	6	4.066204	-0.123131	-0.942281
	6	2.810944	-1.365205	1.456994
	6	-2.417841	-1.659972	-1.383047
	6	-4.007621	-0.453128	0.807962
	8	5.077787	0.143413	-1.471493
	8	3.034080	-1.886352	2.481271
	8	-2.516267	-2.303465	-2.355244
	8	-5.088145	-0.326197	1.244645
	6	1.507435	-1.570832	-1.239877
	8	0.910185	-2.244813	-1.987963
	6	-1.276636	-1.425512	1.384681
	8	-0.643704	-1.945777	2.221498
	15	1.480787	1.394824	0.299222
	15	-1.710317	1.400114	-0.441882
$[(Me_2P)_2CH_2]Ni_2(CO)_6$	6	0.882600	1.682045	2.026695
S-PMe-16-3S(*C*$_1$)	1	1.741692	1.549022	2.707773
	1	0.470869	2.698306	2.164828
	1	0.123121	0.928394	2.294317
	6	2.595781	2.859084	0.068111
	1	2.099081	3.808204	0.343349
	1	3.494313	2.724570	0.695419
	1	2.923510	2.910860	-0.984796
	6	0.054873	1.916637	-0.803630
	1	0.298477	1.511435	-1.804168
	1	0.056817	3.022672	-0.887560
	6	-2.499368	1.973253	-2.019154
	1	-3.595579	1.887585	-1.919320
	1	-2.236669	3.020705	-2.258310
	1	-2.181628	1.318951	-2.849188
	6	-2.275869	2.721520	0.728820
	1	-1.975286	3.731188	0.391852
	1	-3.377447	2.676957	0.791847
	1	-1.874933	2.535755	1.738568

	28	-1.318675	-0.764058	0.087277
	28	1.318677	-0.764046	0.087282
	6	-2.601166	-1.486114	1.108580
	6	-1.474747	-1.480779	-1.567553
	6	2.601179	-1.486108	1.108568
	8	-3.480908	-1.942125	1.734362
	8	-1.677951	-1.940018	-2.627372
	8	3.480934	-1.942121	1.734332
	6	0.000000	-0.570803	1.490664
	8	-0.000003	-0.317972	2.659556
	6	1.474764	-1.480772	-1.567546
	8	1.677975	-1.940018	-2.627360
	15	1.568671	1.462717	-0.200068
	15	-1.568681	1.462703	-0.200082
	6	-1.973737	2.465898	1.302630
$[(Me_2P)_2CH_2]Ni_2(CO)_5$	1	-1.950044	3.552338	1.099043
S-PMe-15-1S(*C*$_S$)	1	-2.984631	2.185793	1.647973
	1	-1.267837	2.225092	2.115748
	6	-2.822146	2.081641	-1.415318
	1	-3.827618	1.774462	-1.077623
	1	-2.796762	3.182290	-1.517768
	1	-2.638460	1.617353	-2.399727
	6	-0.000007	2.254253	-0.845184
	1	-0.000010	3.350862	-0.685012
	1	-0.000002	2.069044	-1.937080
	6	1.973702	2.465926	1.302642
	1	2.984602	2.185843	1.647988
	1	1.949986	3.552364	1.099050
	1	1.267806	2.225106	2.115760
	6	2.822136	2.081673	-1.415295
	1	2.796737	3.182322	-1.517741
	1	3.827611	1.774508	-1.077595
	1	2.638463	1.617387	-2.399708

	15	-1.034660	1.718414	-0.159986
	15	-0.066663	-1.414883	-0.004246
$[(Me_2P)_2CH_2]Ni_2(CO)_5$	28	-1.988882	-0.287100	0.034556
S-PMe-15-2S(*C*$_1$)	28	1.921406	0.159964	-0.018791
	6	-2.763187	-0.536670	1.621740
	6	-2.897862	-0.722518	-1.429251

	6	2.563139	-1.364115	0.672693
	6	2.924806	0.252308	-1.537578
	6	2.340760	1.343742	1.303619
	8	-3.295866	-0.697824	2.659223
	8	-3.511348	-1.010913	-2.392544
	8	3.504433	0.343753	-2.545248
	8	3.142708	-2.286209	1.103393
	8	2.659984	2.118664	2.114599
	6	0.630485	1.502248	-0.938809
	1	0.441855	1.078692	-1.943511
	1	1.153216	2.471544	-1.066912
	6	-1.778683	3.022262	-1.259170
	1	-2.766467	3.312309	-0.858873
	1	-1.138257	3.921369	-1.328451
	1	-1.929740	2.603766	-2.269189
	6	-0.728319	2.702344	1.378388
	1	-1.702201	3.047090	1.769256
	1	-0.267068	2.061985	2.148406
	1	-0.082149	3.581172	1.194634
	6	0.029158	-2.736509	1.309646
	1	0.055615	-2.270060	2.309269
	1	-0.914329	-3.307657	1.229341
	1	0.880386	-3.429749	1.200025
	6	0.290255	-2.439241	-1.517956
	1	-0.532685	-3.169515	-1.635883
	1	0.301742	-1.789071	-2.409040
	1	1.246632	-2.987883	-1.452319

$[(Me_2P)_2CH_2]Ni_2(CO)_5$ **S-PMe-15-1T(*C*$_1$)**	28	-1.522592	-0.551071	-0.065865
	28	1.196286	-0.831095	0.070988
	6	-1.621226	-2.263268	0.601935
	6	-3.276709	-0.351330	-0.575828
	6	2.372106	-2.075676	-0.463533
	8	-1.749661	-3.362534	0.985279
	8	-4.285793	-0.324417	-1.183702
	8	3.138177	-2.888984	-0.821621
	6	0.897296	-0.980032	1.847769
	8	0.849695	-1.055229	3.023176
	6	-0.065150	-0.821814	-1.398784
	8	-0.104436	-0.871271	-2.595874
	15	1.894163	1.263423	-0.261797
	15	-1.131607	1.702842	0.264968

	6	-0.978152	2.210739	2.038701
	1	-0.736196	3.285574	2.136017
	1	-1.937144	2.006920	2.546478
	1	-0.202911	1.603926	2.535407
	6	-2.420051	2.873499	-0.363707
	1	-3.384147	2.644776	0.123052
	1	-2.152112	3.925670	-0.158058
	1	-2.546105	2.734431	-1.451494
	6	0.414950	2.376756	-0.533475
	1	0.611936	3.418718	-0.214195
	1	0.212529	2.385746	-1.621873
	6	2.838907	2.136629	1.070607
	1	3.777526	1.585287	1.254966
	1	3.079372	3.179866	0.793313
	1	2.257153	2.131393	2.008296
	6	2.924274	1.615019	-1.757918
	1	3.083925	2.698376	-1.911282
	1	3.903726	1.118907	-1.639222
	1	2.429372	1.183414	-2.645077
$[(Me_2P)_2CH_2]Ni_2(CO)_5$ **S-PMe-15-2T(*C1*)**	28	-1.425481	-0.417509	-0.474586
	28	1.324302	-0.755921	0.094799
	6	-2.358841	-1.842845	0.129310
	6	-2.268130	0.450956	-1.803062
	6	0.779891	-2.111664	1.183307
	6	3.117575	-1.115199	0.018114
	8	-3.022150	-2.755288	0.449507
	8	-2.754058	0.979137	-2.734453
	8	0.519106	-3.019915	1.879357
	8	4.208052	-1.452163	-0.276271
	15	-1.244888	1.160922	1.137348
	15	1.490204	1.512064	-0.129260
	6	0.106923	-1.048903	-1.472245
	8	0.405083	-1.459799	-2.556436
	6	-2.722878	2.260415	1.342945
	1	-3.574689	1.651029	1.692803
	1	-2.537925	3.073578	2.069122
	1	-2.996181	2.693789	0.365403
	6	-0.894971	0.680245	2.890718
	1	-0.936888	1.554044	3.567564
	1	-1.639787	-0.067589	3.214354
	1	0.102255	0.211004	2.945869

	6	0.120770	2.396725	0.783051
	1	0.511100	2.839225	1.719216
	1	-0.283848	3.217078	0.160865
	6	1.357556	2.179131	-1.847722
	1	1.431883	3.281954	-1.864156
	1	2.163554	1.747543	-2.466294
	1	0.391913	1.867043	-2.280767
	6	3.030688	2.312722	0.506207
	1	3.178122	2.038767	1.565098
	1	3.896417	1.935518	-0.065903
	1	2.987570	3.412999	0.412170

	28	-1.209123	-0.768179	0.010668
	28	1.209137	-0.768171	0.010654
	6	-2.656819	-1.788951	-0.013305
	6	2.656848	-1.788921	-0.013327
	8	-3.637486	-2.435219	-0.042110
	8	3.637521	-2.435181	-0.042135
	6	0.000023	-1.389040	1.397832
	8	0.000015	-1.936326	2.449192
	6	0.000011	-1.176589	-1.458039
	8	-0.000015	-1.542418	-2.584450
$[(Me_2P)_2CH_2]Ni_2(CO)_4$	15	1.548820	1.474353	-0.033541
S-PMe-14-1S(*C*$_S$)	15	-1.548838	1.474337	-0.033546
	6	1.991965	2.282425	1.576735
	1	2.960211	1.877029	1.919390
	1	2.072660	3.381227	1.483646
	1	1.237245	2.033858	2.342435
	6	2.822919	2.198755	-1.169563
	1	2.822298	3.304238	-1.152130
	1	3.819433	1.833487	-0.864481
	1	2.635400	1.848839	-2.199601
	6	-0.000013	2.382964	-0.560268
	1	-0.000010	2.373563	-1.667588
	1	-0.000018	3.439305	-0.228499

	6	-1.992019	2.282427	1.576711
	1	-2.072737	3.381225	1.483601
	1	-2.960260	1.877016	1.919361
	1	-1.237302	2.033891	2.342425
	6	-2.822939	2.198694	-1.169594
	1	-3.819448	1.833411	-0.864515
	1	-2.822341	3.304178	-1.152182
	1	-2.635403	1.848763	-2.199625

	15	-1.199044	1.452725	-0.667648
	15	0.185766	-1.528215	-0.658048
	28	-1.164657	-0.375494	0.678452
	28	1.514512	0.234511	-0.266427
	6	-0.595054	0.077346	2.313147
	6	-2.694180	-1.287674	0.744451
	6	2.855298	-0.863073	0.131751
	6	2.189920	1.777750	0.321485
	8	-0.291311	0.363480	3.412201
	8	-3.708322	-1.882504	0.763503
	8	3.806194	-1.517819	0.331324
$[(Me_2P)_2CH_2]Ni_2(CO)_4$	8	2.682719	2.794724	0.620094
S-PMe-14-2S(*C*$_1$)	6	-2.541128	1.748689	-1.920664
	1	-3.494288	1.945389	-1.397255
	1	-2.303632	2.606248	-2.577347
	1	-2.674260	0.844598	-2.539633
	6	-1.117826	3.110296	0.153813
	1	-0.963276	3.922821	-0.580328
	1	-2.061116	3.289086	0.699370
	1	-0.295771	3.122582	0.889051
	6	0.841891	-3.180907	-0.127706
	1	0.002440	-3.900860	-0.141484
	1	1.642908	-3.556544	-0.789653
	1	1.218498	-3.114093	0.906300

	6	-0.253405	-1.915735	-2.418350
	1	0.631587	-2.255498	-2.986003
	1	-1.005919	-2.726539	-2.413835
	1	-0.696794	-1.042483	-2.922248
	6	0.383895	1.335836	-1.600748
	1	0.804459	2.320857	-1.872542
	1	0.267687	0.746087	-2.525685

$[(Me_2P)_2CH_2]Ni_2(CO)_4$ **S-PMe-14-1T(C_S/C_1)**	28	-1.159997	-0.860698	0.023503
	28	1.159978	-0.860706	0.023531
	6	-2.749903	-1.660853	0.066335
	6	2.749875	-1.660880	0.066350
	8	-3.820319	-2.149722	0.095685
	8	3.820287	-2.149758	0.095690
	6	-0.000013	-0.999380	1.597980
	8	-0.000043	-1.024445	2.792622
	6	0.000003	-1.177685	-1.527197
	8	0.000024	-1.378649	-2.704437
	15	1.554950	1.325544	-0.094259
	15	-1.554928	1.325559	-0.094269
	6	1.989116	2.198289	1.478208
	1	2.974224	1.836750	1.821428
	1	2.029299	3.295635	1.345530
	1	1.251804	1.944427	2.258579
	6	2.833754	1.960483	-1.268338
	1	2.849680	3.065613	-1.305272
	1	3.824885	1.595207	-0.946644
	1	2.633322	1.558763	-2.276399
	6	0.000017	2.195194	-0.675748
	1	0.000021	2.101574	-1.779233
	1	0.000019	3.274825	-0.425456
	6	-1.989073	2.198296	1.478208
	1	-2.029219	3.295646	1.345546

	1	-2.974193	1.836785	1.821422
	1	-1.251771	1.944400	2.258578
	6	-2.833723	1.960534	-1.268341
	1	-3.824859	1.595272	-0.946648
	1	-2.849628	3.065664	-1.305264
	1	-2.633298	1.558819	-2.276405

	15	-0.955794	1.321393	-1.102567
	15	0.430157	-1.641527	0.178586
	28	-1.357690	-0.318619	0.419930
	28	1.646625	0.290307	0.093121
	6	-1.625551	0.348274	2.073336
	6	-2.653695	-1.361436	-0.230060
	6	3.192361	-0.258204	-0.658494
	6	1.671189	1.677613	1.276660
	8	-1.856501	0.755130	3.149537
	8	-3.460952	-2.087654	-0.681347
	8	4.133234	-0.675276	-1.221396
	8	1.770564	2.579291	2.017850
$[(Me_2P)_2CH_2]Ni_2(CO)_4$	6	-1.961451	1.274037	-2.666916
S-PMe-14-2T(*C*$_1$)	1	-3.030444	1.400679	-2.418832
	1	-1.648796	2.068287	-3.368999
	1	-1.835523	0.290211	-3.150713
	6	-1.167393	3.075602	-0.557072
	1	-0.905622	3.783142	-1.365183
	1	-2.217332	3.237181	-0.256740
	1	-0.527561	3.270864	0.319658
	6	0.941625	-2.797843	1.534093
	1	0.220698	-3.633399	1.616013
	1	1.947792	-3.216667	1.343982
	1	0.954982	-2.252490	2.492574
	6	0.532161	-2.743362	-1.308336
	1	1.547531	-3.167643	-1.416602

	1	-0.192378	-3.574329	-1.221746
	1	0.290445	-2.165467	-2.216694
	6	0.781267	1.181759	-1.593409
	1	1.311448	2.131789	-1.773424
	1	0.925299	0.472033	-2.424964
	28	2.252937	-0.694012	0.000000
	28	-2.252937	0.694012	0.000000
	6	3.567818	-1.897372	0.000000
	6	-3.567818	1.897372	0.000000
	8	4.456997	-2.671290	0.000000
	8	-4.456997	2.671290	0.000000
	15	1.093533	-1.199133	1.860050
	15	-1.093533	1.199133	1.860050
	15	1.093533	-1.199133	-1.860050
	15	-1.093533	1.199133	-1.860050
	6	-2.851977	-0.977972	0.000000
	8	-3.326165	-2.059822	0.000000
	6	2.851977	0.977972	0.000000
	8	3.326165	2.059822	0.000000
	6	0.000000	0.000000	-2.799838
	1	-0.660279	-0.597758	-3.458674
	1	0.660279	0.597758	-3.458674
	6	2.238530	-1.662468	-3.249073
	1	2.820968	-2.551828	-2.950820
	1	1.689332	-1.886556	-4.183083
	1	2.949782	-0.837826	-3.429407
	6	0.000000	-2.697390	-1.828794
	1	-0.313191	-2.986858	-2.849696
	1	0.549589	-3.537669	-1.370069
	1	-0.898938	-2.495599	-1.224035
	6	-2.238530	1.662468	-3.249073
	1	-2.820968	2.551828	-2.950820
	1	-1.689332	1.886556	-4.183083
	1	-2.949782	0.837826	-3.429407
	6	0.000000	2.697390	-1.828794
	1	0.313191	2.986858	-2.849696
	1	-0.549589	3.537669	-1.370069
	1	0.898938	2.495599	-1.224035
	6	0.000000	2.697390	1.828794
	1	-0.549589	3.537669	1.370069
	1	0.313191	2.986858	2.849696
	1	0.898938	2.495599	1.224035

$[(Me_2P)_2CH_2]_2Ni_2(CO)_4$
S-PMe-24-1S(C_{2h})

	6	-2.238530	1.662468	3.249073
	1	-1.689332	1.886556	4.183083
	1	-2.820968	2.551828	2.950820
	1	-2.949782	0.837826	3.429407
	6	0.000000	0.000000	2.799838
	1	-0.660279	-0.597758	3.458674
	1	0.660279	0.597758	3.458674
	6	2.238530	-1.662468	3.249073
	1	1.689332	-1.886556	4.183083
	1	2.820968	-2.551828	2.950820
	1	2.949782	-0.837826	3.429407
	6	0.000000	-2.697390	1.828794
	1	0.549589	-3.537669	1.370069
	1	-0.313191	-2.986858	2.849696
	1	-0.898938	-2.495599	1.224035
	28	0.000000	2.329305	0.446429
	28	0.000000	-2.329305	0.446429
	6	0.000000	1.841200	2.167851
	6	0.000000	4.097957	0.255450
	6	0.000000	-1.841200	2.167851
	6	0.000000	-4.097957	0.255450
	8	0.000000	1.637962	3.326125
	8	0.000000	5.273932	0.161437
	8	0.000000	-5.273932	0.161437
	8	0.000000	-1.637962	3.326125
	15	1.872551	1.642922	-0.553323
	15	1.872551	-1.642922	-0.553323
$[(Me_2P)_2CH_2]_2Ni_2(CO)_4$	15	-1.872551	1.642922	-0.553323
S-PMe-24-2S(C_{2v})	15	-1.872551	-1.642922	-0.553323
	6	-3.366928	1.753873	0.541115
	1	-3.470865	2.805810	0.861161
	1	-4.294638	1.437415	0.028250
	1	-3.218534	1.144976	1.447802
	6	-2.422568	2.740751	-1.951381
	1	-3.416686	2.455250	-2.344699
	1	-2.463167	3.782509	-1.588158
	1	-1.684655	2.698871	-2.771942
	6	-2.118229	0.000000	-1.424084
	1	-1.389514	0.000000	-2.259685
	1	-3.132397	0.000000	-1.878074
	6	-2.422568	-2.740751	-1.951381
	1	-2.463167	-3.782509	-1.588158

	1	-3.416686	-2.455250	-2.344699
	1	-1.684655	-2.698871	-2.771942
	6	-3.366928	-1.753873	0.541115
	1	-4.294638	-1.437415	0.028250
	1	-3.470865	-2.805810	0.861161
	1	-3.218534	-1.144976	1.447802
	6	3.366928	-1.753873	0.541115
	1	3.470865	-2.805810	0.861161
	1	4.294638	-1.437415	0.028250
	1	3.218534	-1.144976	1.447802
	6	2.422568	-2.740751	-1.951381
	1	3.416686	-2.455250	-2.344699
	1	2.463167	-3.782509	-1.588158
	1	1.684655	-2.698871	-2.771942
	6	2.118229	0.000000	-1.424084
	1	1.389514	0.000000	-2.259685
	1	3.132397	0.000000	-1.878074
	6	3.366928	1.753873	0.541115
	1	4.294638	1.437415	0.028250
	1	3.470865	2.805810	0.861161
	1	3.218534	1.144976	1.447802
	6	2.422568	2.740751	-1.951381
	1	2.463167	3.782509	-1.588158
	1	3.416686	2.455250	-2.344699
	1	1.684655	2.698871	-2.771942
	28	0.575243	2.149109	0.000000
	28	-0.022504	-1.966115	0.000000
	6	0.632679	3.931833	0.000000
	6	1.597512	-2.837371	0.000000
	6	-1.845518	-2.224892	0.000000
	8	0.691001	5.109461	0.000000
	8	-2.882516	-2.814960	0.000000
	8	2.396126	-3.717644	0.000000
$[(Me_2P)_2CH_2]_2Ni_2(CO)_4$	15	-0.507628	1.585155	-1.876517
S-PMe-24-1T(*C*$_S$)	15	0.074271	-1.538357	-2.278631
	15	-0.507628	1.585155	1.876517
	15	0.074271	-1.538357	2.278631
	6	2.176451	1.362205	0.000000
	8	3.263432	0.907230	0.000000
	6	-0.492372	2.945981	3.141880
	1	-0.994649	3.833289	2.717861
	1	-1.001170	2.653273	4.079711

	1	0.552102	3.226024	3.364041
	6	-2.310598	1.147285	1.884457
	1	-2.687329	0.954364	2.906604
	1	-2.878952	1.987590	1.447671
	1	-2.472421	0.255309	1.252870
	6	0.248888	0.219565	2.907598
	1	-0.131218	0.265635	3.949127
	1	1.333228	0.439027	2.931768
	6	-1.381202	-2.148543	3.253015
	1	-1.480109	-3.236716	3.096006
	1	-1.259839	-1.944939	4.332964
	1	-2.307787	-1.671477	2.892650
	6	1.475331	-2.347302	3.183060
	1	1.456289	-2.100622	4.260397
	1	1.404211	-3.441876	3.058782
	1	2.433822	-2.016358	2.747891
	6	0.248888	0.219565	-2.907598
	1	-0.131218	0.265635	-3.949127
	1	1.333228	0.439027	-2.931768
	6	-2.310598	1.147285	-1.884457
	1	-2.878952	1.987590	-1.447671
	1	-2.687329	0.954364	-2.906604
	1	-2.472421	0.255309	-1.252870
	6	-0.492372	2.945981	-3.141880
	1	-1.001170	2.653273	-4.079711
	1	-0.994649	3.833289	-2.717861
	1	0.552102	3.226024	-3.364041
	6	1.475331	-2.347302	-3.183060
	1	1.404211	-3.441876	-3.058782
	1	1.456289	-2.100622	-4.260397
	1	2.433822	-2.016358	-2.747891
	6	-1.381202	-2.148543	-3.253015
	1	-1.259839	-1.944939	-4.332964
	1	-1.480109	-3.236716	-3.096006
	1	-2.307787	-1.671477	-2.892650
	28	0.000000	0.000000	-2.146531
	28	0.000000	0.000000	2.271749
$[(Me_2P)_2CH_2]_2Ni_2(CO)_4$	6	-1.307333	-1.110431	-2.834793
S-PMe-24-2T(*C*$_2$)	6	1.307333	1.110431	-2.834793
	6	0.000000	-1.512296	3.215703
	6	0.000000	1.512296	3.215703
	8	-1.935421	-1.622295	-3.711590

8	1.935421	1.622295	-3.711590
8	-0.003554	2.499784	3.860362
8	0.003554	-2.499784	3.860362
15	-1.397158	1.625867	-1.390760
15	-2.012188	-0.050134	1.243864
15	1.397158	-1.625867	-1.390760
15	2.012188	0.050134	1.243864
6	0.614634	-3.130589	-0.655086
1	-0.168199	-3.509801	-1.334438
1	1.364188	-3.924094	-0.476109
1	0.144421	-2.852478	0.303643
6	2.517689	-2.352964	-2.675972
1	3.229509	-3.080494	-2.243359
1	1.900964	-2.858401	-3.439947
1	3.076380	-1.541645	-3.173797
6	2.621244	-1.157330	-0.061626
1	3.511925	-0.720453	-0.553574
1	2.945739	-2.082560	0.454309
6	2.599762	1.651037	0.519544
1	2.342688	2.477271	1.205416
1	3.694185	1.640001	0.358432
1	2.095773	1.810393	-0.451400
6	3.327177	-0.239986	2.526245
1	4.344095	-0.216791	2.090987
1	3.247535	0.544682	3.298924
1	3.159157	-1.214389	3.017045
6	-2.599762	-1.651037	0.519544
1	-2.342688	-2.477271	1.205416
1	-3.694185	-1.640001	0.358432
1	-2.095773	-1.810393	-0.451400
6	-3.327177	0.239986	2.526245
1	-4.344095	0.216791	2.090987
1	-3.247535	-0.544682	3.298924
1	-3.159157	1.214389	3.017045
6	-2.621244	1.157330	-0.061626
1	-2.945739	2.082560	0.454309
1	-3.511925	0.720453	-0.553574
6	-2.517689	2.352964	-2.675972
1	-3.229509	3.080494	-2.243359
1	-1.900964	2.858401	-3.439947
1	-3.076380	1.541645	-3.173797
6	-0.614634	3.130589	-0.655086
1	0.168199	3.509801	-1.334438
1	-1.364188	3.924094	-0.476109

	1	-0.144421	2.852478	0.303643

	28	0.000000	1.707675	0.395012
	28	0.000000	-1.707675	0.395012
	6	0.000000	1.235826	2.204650
	6	0.000000	3.491457	0.750953
	6	0.000000	-1.235826	2.204650
	6	0.000000	-3.491457	0.750953
	8	0.000000	1.484121	3.366233
	8	0.000000	4.554098	1.273285
	8	0.000000	-4.554098	1.273285
	8	0.000000	-1.484121	3.366233
	15	1.943772	1.557834	-0.705435
	15	1.943772	-1.557834	-0.705435
	15	-1.943772	1.557834	-0.705435
	15	-1.943772	-1.557834	-0.705435
	6	-3.434607	1.864862	0.356018
	1	-3.349811	2.880411	0.781563
	1	-4.380794	1.786440	-0.211734
	1	-3.447465	1.154786	1.199572
	6	-2.225684	2.820112	-2.039817
$[(Me_2P)_2CH_2]_2Ni_2(CO)_4$	1	-3.230028	2.730947	-2.495074
S-PMe-24-3T(C_{2v})	1	-2.114651	3.828157	-1.603124
	1	-1.458867	2.706156	-2.826014
	6	-2.402639	0.000000	-1.625425
	1	-1.787384	0.000000	-2.546890
	1	-3.469394	0.000000	-1.932423
	6	-2.225684	-2.820112	-2.039817
	1	-2.114651	-3.828157	-1.603124
	1	-3.230028	-2.730947	-2.495074
	1	-1.458867	-2.706156	-2.826014
	6	-3.434607	-1.864862	0.356018
	1	-4.380794	-1.786440	-0.211734
	1	-3.349811	-2.880411	0.781563
	1	-3.447465	-1.154786	1.199572
	6	3.434607	-1.864862	0.356018
	1	3.349811	-2.880411	0.781563
	1	4.380794	-1.786440	-0.211734
	1	3.447465	-1.154786	1.199572
	6	2.225684	-2.820112	-2.039817
	1	3.230028	-2.730947	-2.495074
	1	2.114651	-3.828157	-1.603124

	1	1.458867	-2.706156	-2.826014
	6	2.402639	0.000000	-1.625425
	1	1.787384	0.000000	-2.546890
	1	3.469394	0.000000	-1.932423
	6	3.434607	1.864862	0.356018
	1	4.380794	1.786440	-0.211734
	1	3.349811	2.880411	0.781563
	1	3.447465	1.154786	1.199572
	6	2.225684	2.820112	-2.039817
	1	2.114651	3.828157	-1.603124
	1	3.230028	2.730947	-2.495074
	1	1.458867	2.706156	-2.826014
	28	-0.005586	0.597503	1.340409
	28	-0.005586	0.597503	-1.340409
	6	-0.096946	1.726612	2.710103
	6	-0.096946	1.726612	-2.710103
	8	-0.161193	2.424370	3.659404
	8	-0.161193	2.424370	-3.659404
	15	-1.917011	-0.549759	1.518231
	15	-1.917011	-0.549759	-1.518231
	15	1.782625	-0.736553	1.556014
	15	1.782625	-0.736553	-1.556014
	6	0.681139	1.782226	0.000000
	8	1.353040	2.776484	0.000000
	6	1.903720	-2.096226	2.822270
	1	2.883460	-2.608945	2.792580
$[(Me_2P)_2CH_2]_2Ni_2(CO)_3$	1	1.757873	-1.661061	3.826869
S-PMe-23-1S(*C*$_S$)	1	1.104553	-2.839402	2.653364
	6	3.349615	0.187393	1.932286
	1	3.267029	0.611503	2.948887
	1	4.246890	-0.457451	1.879444
	1	3.457453	1.033677	1.232814
	6	2.235212	-1.677878	0.000000
	1	1.607581	-2.591132	0.000000
	1	3.297067	-1.997003	0.000000
	6	1.903720	-2.096226	-2.822270
	1	1.757873	-1.661061	-3.826869
	1	2.883460	-2.608945	-2.792580
	1	1.104553	-2.839402	-2.653364
	6	3.349615	0.187393	-1.932286
	1	4.246890	-0.457451	-1.879444
	1	3.267029	0.611503	-2.948887

	1	3.457453	1.033677	-1.232814
	6	-2.425019	-1.508495	0.000000
	1	-1.804050	-2.426189	0.000000
	1	-3.492239	-1.810296	0.000000
	6	-2.131286	-1.846518	2.839777
	1	-1.932980	-1.389037	3.825320
	1	-3.150540	-2.276379	2.842523
	1	-1.399511	-2.659724	2.689135
	6	-3.415055	0.490731	1.870763
	1	-4.352724	-0.095960	1.851622
	1	-3.292572	0.944210	2.870444
	1	-3.477811	1.315055	1.141020
	6	-3.415055	0.490731	-1.870763
	1	-3.292572	0.944210	-2.870444
	1	-4.352724	-0.095960	-1.851622
	1	-3.477811	1.315055	-1.141020
	6	-2.131286	-1.846518	-2.839777
	1	-3.150540	-2.276379	-2.842523
	1	-1.932980	-1.389037	-3.825320
	1	-1.399511	-2.659724	-2.689135

	28	-2.299843	0.043952	-0.235601
	28	2.395528	-0.118387	-0.342453
	6	-3.741461	-0.137333	-1.215843
	6	2.743977	0.443473	-1.995089
	6	3.782880	-0.661888	0.632887
	8	-4.746030	-0.239666	-1.832546
	8	4.709515	-1.018689	1.270179
	8	2.985204	0.810839	-3.089779
	15	-1.758499	-1.691160	1.013353
	15	1.028195	-1.879143	-0.520799
$[(Me_2P)_2CH_2]_2Ni_2(CO)_3$	15	-1.526412	2.104855	-0.144757
S-PMe-23-2S(*C*$_1$)	15	1.530655	1.620644	0.759998
	6	-2.103767	3.181521	-1.547739
	1	-3.205678	3.136682	-1.598037
	1	-1.782838	4.234057	-1.430594
	1	-1.706096	2.784311	-2.497990
	6	-2.272843	3.014766	1.298527
	1	-2.068922	4.100905	1.244990
	1	-3.365036	2.853327	1.291811
	1	-1.875029	2.617038	2.247196
	6	0.255447	2.702690	-0.073117
	1	0.266311	3.716803	0.377939

	1	0.598698	2.805332	-1.120341
	6	0.827932	1.404497	2.463975
	1	1.563069	0.864063	3.086034
	1	0.588051	2.370897	2.945905
	1	-0.089107	0.792925	2.391226
	6	2.844013	2.893040	1.087757
	1	2.456994	3.767679	1.644165
	1	3.659680	2.423747	1.665430
	1	3.267184	3.229410	0.125094
	6	-0.169695	-1.912175	-1.935528
	1	0.380939	-1.667365	-2.860823
	1	-0.663830	-2.894416	-2.056039
	1	-0.947778	-1.130978	-1.781017
	6	1.963936	-3.455627	-0.818026
	1	1.289434	-4.319073	-0.972399
	1	2.601874	-3.327492	-1.710007
	1	2.625566	-3.656887	0.042529
	6	-0.015934	-2.388405	0.960416
	1	0.525014	-2.022230	1.852204
	1	-0.065915	-3.493293	1.029707
	6	-2.740380	-3.212077	0.585507
	1	-2.484334	-4.077049	1.226880
	1	-3.814288	-2.979304	0.692875
	1	-2.562498	-3.475455	-0.471498
	6	-2.066345	-1.624874	2.848086
	1	-3.126413	-1.369436	3.023820
	1	-1.846325	-2.593341	3.334822
	1	-1.443079	-0.840135	3.311022
	28	1.035086	-0.998859	0.159948
	28	-0.790549	1.053683	0.525892
	6	2.260846	-2.339616	0.271658
	6	-1.094041	2.378525	1.671801
	8	3.025245	-3.167760	0.655685
	8	-1.254664	3.222548	2.484239
$[(Me_2P)_2CH_2]_2Ni_2(CO)_3$	15	-0.637586	-2.345512	-0.597985
S-PMe-23-1T(*C*$_1$)	15	-2.636422	-0.021363	-0.054874
	15	2.581350	0.673236	0.057845
	15	0.197110	1.952944	-1.255990
	6	-0.013861	-0.292841	1.658703
	8	-0.131023	-0.686668	2.795108
	6	4.280349	0.286187	-0.573731
	1	4.939433	1.173302	-0.551421

	1	4.721535	-0.508376	0.053483
	1	4.212650	-0.097098	-1.606585
	6	2.947316	1.468180	1.689431
	1	3.340215	0.703287	2.381930
	1	3.679806	2.291130	1.592950
	1	2.002622	1.856176	2.107576
	6	2.047044	2.124916	-0.993535
	1	2.600330	2.132665	-1.952754
	1	2.252333	3.077759	-0.469752
	6	0.164182	1.137285	-2.928651
	1	-0.883617	1.002381	-3.252527
	1	0.700321	1.732509	-3.692378
	1	0.630846	0.140046	-2.838313
	6	-0.265340	3.692952	-1.731282
	1	0.389252	4.102166	-2.523945
	1	-1.310872	3.706804	-2.088097
	1	-0.206892	4.337732	-0.837171
	6	-2.277336	-1.569074	-1.051621
	1	-2.178360	-1.243128	-2.105471
	1	-3.102497	-2.308495	-1.002873
	6	-0.296811	-3.416586	-2.074234
	1	0.617584	-4.002832	-1.875247
	1	-1.133753	-4.106484	-2.292008
	1	-0.107043	-2.781484	-2.957179
	6	-1.109071	-3.615191	0.667929
	1	-1.939207	-4.261495	0.327553
	1	-0.223076	-4.238858	0.880671
	1	-1.388847	-3.108716	1.607273
	6	-3.656964	-0.672942	1.351646
	1	-4.085400	0.186303	1.897559
	1	-4.477236	-1.333046	1.012300
	1	-3.006690	-1.218048	2.057094
	6	-3.966207	0.752552	-1.100645
	1	-4.793141	0.051589	-1.322906
	1	-4.371571	1.628318	-0.563550
	1	-3.529650	1.110223	-2.049763
	28	1.476231	-0.164742	0.000000
	28	-1.105373	0.213688	0.000000
$[(Me_2P)_2CH_2]_2Ni_2(CO)_3$	6	3.256086	-0.485541	0.000000
S-PMe-23-2T(*C*$_S$)	8	4.355432	-0.932357	0.000000
	15	1.256479	0.187656	2.297467
	15	-1.837999	-0.234207	2.027990

15	1.256479	0.187656	-2.297467
15	-1.837999	-0.234207	-2.027990
6	-0.004253	-1.409143	0.000000
8	-0.171652	-2.608126	0.000000
6	-0.769954	1.959336	0.000000
8	-0.637864	3.142160	0.000000
6	-0.288016	-0.573281	-3.039227
1	-0.121363	-1.667259	-3.003843
1	-0.409997	-0.282955	-4.101458
6	1.243207	1.922459	-2.960207
1	2.212402	2.394475	-2.719784
1	1.092755	1.942389	-4.056226
1	0.453063	2.508895	-2.462885
6	2.567610	-0.582405	-3.365119
1	2.377115	-0.425603	-4.442907
1	3.546323	-0.142789	-3.103759
1	2.617190	-1.665194	-3.155669
6	-2.861337	-1.724995	-2.452877
1	-3.886846	-1.579631	-2.068903
1	-2.907485	-1.908494	-3.543077
1	-2.425446	-2.605231	-1.948638
6	-2.676734	1.083338	-3.031564
1	-2.825344	0.777190	-4.084348
1	-3.657582	1.309966	-2.577692
1	-2.071675	2.005908	-3.000237
6	-2.676734	1.083338	3.031564
1	-3.657582	1.309966	2.577692
1	-2.825344	0.777190	4.084348
1	-2.071675	2.005908	3.000237
6	-2.861337	-1.724995	2.452877
1	-2.907485	-1.908494	3.543077
1	-3.886846	-1.579631	2.068903
1	-2.425446	-2.605231	1.948638
6	-0.288016	-0.573281	3.039227
1	-0.121363	-1.667259	3.003843
1	-0.409997	-0.282955	4.101458
6	1.243207	1.922459	2.960207
1	1.092755	1.942389	4.056226
1	2.212402	2.394475	2.719784
1	0.453063	2.508895	2.462885
6	2.567610	-0.582405	3.365119
1	3.546323	-0.142789	3.103759
1	2.377115	-0.425603	4.442907
1	2.617190	-1.665194	3.155669

	28	0.000000	0.000000	1.341219
	28	0.000000	0.000000	-1.110077
	6	0.000000	0.000000	3.139470
	8	0.000000	0.000000	4.325720
	15	0.000000	2.413626	1.222450
	15	0.076706	2.031974	-1.894846
	15	0.000000	-2.413626	1.222450
	15	-0.076706	-2.031974	-1.894846
	6	-1.558545	0.039176	-0.069404
	8	-2.757176	0.092840	0.025376
	6	1.558545	-0.039176	-0.069404
	8	2.757176	-0.092840	0.025376
	6	-0.560866	-3.107105	-0.424938
	1	-1.667613	-3.089836	-0.393923
	1	-0.239594	-4.161344	-0.545776
	6	1.648798	-3.221328	1.486226
	1	1.987759	-2.997733	2.513343
	1	1.606493	-4.317999	1.346940
	1	2.387070	-2.785159	0.792089
	6	-1.070218	-3.351815	2.412901
	1	-1.015070	-4.445755	2.260640
	1	-0.749293	-3.114635	3.442778
	1	-2.115818	-3.016655	2.298293
	6	-1.319057	-2.609812	-3.152311
	1	-1.059781	-2.178373	-4.135623
	1	-1.349629	-3.712526	-3.240875
	1	-2.317600	-2.234789	-2.868003
	6	1.455396	-2.880792	-2.517907
	1	1.302244	-3.965230	-2.675505
	1	1.753937	-2.416790	-3.474921
	1	2.279855	-2.724108	-1.801210
	6	1.319057	2.609812	-3.152311
	1	1.059781	2.178373	-4.135623
	1	1.349629	3.712526	-3.240875
	1	2.317600	2.234789	-2.868003
	6	-1.455396	2.880792	-2.517907
	1	-1.302244	3.965230	-2.675505
	1	-1.753937	2.416790	-3.474921
	1	-2.279855	2.724108	-1.801210
	6	0.560866	3.107105	-0.424938
	1	0.239594	4.161344	-0.545776

$[(Me_2P)_2CH_2]_2Ni_2(CO)_3$
S-PMe-23-3T(C_2)

	1	1.667613	3.089836	-0.393923
	6	1.070218	3.351815	2.412901
	1	1.015070	4.445755	2.260640
	1	0.749293	3.114635	3.442778
	1	2.115818	3.016655	2.298293
	6	-1.648798	3.221328	1.486226
	1	-1.987759	2.997733	2.513343
	1	-1.606493	4.317999	1.346940
	1	-2.387070	2.785159	0.792089
	28	0.000000	0.000000	-1.900315
	28	0.000000	0.000000	2.036254
	6	0.000000	0.000000	-3.676512
	6	1.344877	0.714315	2.967437
	6	-1.344877	-0.714315	2.967437
	8	0.000000	0.000000	-4.871865
	8	-2.226852	-1.181894	3.594740
	8	2.226852	1.181894	3.594740
	15	-0.868540	-1.965926	-1.449067
	15	0.967092	-1.788388	1.044449
	15	0.868540	1.965926	-1.449067
	15	-0.967092	1.788388	1.044449
	6	2.632049	2.062714	-0.858805
	1	3.286326	1.553406	-1.587424
	1	2.966109	3.110504	-0.732210
	1	2.709980	1.537908	0.108805
$[(Me_2P)_2CH_2]_2Ni_2(CO)_3$	6	0.887793	3.185335	-2.842955
S-PMe-23-4T(*C*$_2$)	1	1.306310	4.159090	-2.529153
	1	1.499177	2.775333	-3.665583
	1	-0.139420	3.325034	-3.220099
	6	0.000000	2.919937	-0.086670
	1	-0.685064	3.660983	-0.543081
	1	0.740980	3.472220	0.523916
	6	-2.556687	1.608469	0.110521
	1	-3.260304	0.998013	0.704032
	1	-3.014745	2.593939	-0.098249
	1	-2.340585	1.087003	-0.842930
	6	-1.474749	3.000082	2.358641
	1	-1.926571	3.911745	1.924455
	1	-2.208223	2.516921	3.027980
	1	-0.596182	3.279822	2.965730
	6	2.556687	-1.608469	0.110521
	1	3.260304	-0.998013	0.704032

	1	3.014745	-2.593939	-0.098249
	1	2.340585	-1.087003	-0.842930
	6	1.474749	-3.000082	2.358641
	1	1.926571	-3.911745	1.924455
	1	2.208223	-2.516921	3.027980
	1	0.596182	-3.279822	2.965730
	6	0.000000	-2.919937	-0.086670
	1	-0.740980	-3.472220	0.523916
	1	0.685064	-3.660983	-0.543081
	6	-0.887793	-3.185335	-2.842955
	1	-1.306310	-4.159090	-2.529153
	1	-1.499177	-2.775333	-3.665583
	1	0.139420	-3.325034	-3.220099
	6	-2.632049	-2.062714	-0.858805
	1	-3.286326	-1.553406	-1.587424
	1	-2.966109	-3.110504	-0.732210
	1	-2.709980	-1.537908	0.108805

	28	1.292756	0.424196	0.000000
	28	-1.258381	0.495797	0.000000
	6	2.826797	1.300323	0.000000
	6	-0.011945	1.846719	0.000000
	8	3.874860	1.845730	0.000000
	8	-0.116798	3.043209	0.000000
	15	1.201770	-0.751564	1.912657
	15	-1.835181	-0.084553	2.026264
	15	1.201770	-0.751564	-1.912657
	15	-1.835181	-0.084553	-2.026264
	6	1.911236	0.175872	-3.360589
	1	2.971176	0.400697	-3.147694
	1	1.841477	-0.396109	-4.305259
	1	1.385479	1.138934	-3.475334
	6	2.116798	-2.364532	-2.105454
	1	2.015173	-2.784525	-3.124156
	1	3.187394	-2.195829	-1.891979
	1	1.734035	-3.097290	-1.373381
	6	-0.481464	-1.252046	-2.583693
	1	-0.724001	-2.231262	-2.126738
	1	-0.458614	-1.388024	-3.684361
	6	-3.346528	-1.054196	-2.534914
	1	-4.242577	-0.429423	-2.369525
	1	-3.318685	-1.365393	-3.596697
	1	-3.438193	-1.950908	-1.896777

$[(Me_2P)_2CH_2]_2Ni_2(CO)_2$
S-PMe-22-1S(C_S)

	6	-1.843145	1.230993	-3.339342
	1	-1.882485	0.806136	-4.359847
	1	-2.723846	1.879766	-3.185902
	1	-0.944610	1.861656	-3.231551
	6	-1.843145	1.230993	3.339342
	1	-2.723846	1.879766	3.185902
	1	-1.882485	0.806136	4.359847
	1	-0.944610	1.861656	3.231551
	6	-3.346528	-1.054196	2.534914
	1	-3.318685	-1.365393	3.596697
	1	-4.242577	-0.429423	2.369525
	1	-3.438193	-1.950908	1.896777
	6	-0.481464	-1.252046	2.583693
	1	-0.724001	-2.231262	2.126738
	1	-0.458614	-1.388024	3.684361
	6	1.911236	0.175872	3.360589
	1	1.841477	-0.396109	4.305259
	1	2.971176	0.400697	3.147694
	1	1.385479	1.138934	3.475334
	6	2.116798	-2.364532	2.105454
	1	3.187394	-2.195829	1.891979
	1	2.015173	-2.784525	3.124156
	1	1.734035	-3.097290	1.373381
	28	0.622533	1.350971	0.000000
	28	-0.622533	-1.350971	0.000000
	6	2.314439	1.818633	0.000000
	6	-2.314439	-1.818633	0.000000
	8	3.433223	2.211792	0.000000
	8	-3.433223	-2.211792	0.000000
	15	-0.432487	1.448859	1.930936
	15	0.432487	-1.448859	1.930936
	15	-0.432487	1.448859	-1.930936
	15	0.432487	-1.448859	-1.930936
	6	-2.285765	1.471759	-2.054942
	1	-2.677563	2.319476	-1.464899
	1	-2.637541	1.564951	-3.100388
	1	-2.673482	0.537545	-1.612924
	6	0.000000	2.905698	-3.003909
	1	-0.474460	2.844281	-4.001538
	1	-0.333045	3.834087	-2.506381
	1	1.096583	2.957760	-3.118056
	6	0.000000	0.000000	-3.036414

$[(Me_2P)_2CH_2]_2Ni_2(CO)_2$
S-PMe-22-2S(*C_{2h}*)

	1	0.853983	0.270537	-3.686233
	1	-0.853983	-0.270537	-3.686233
	6	2.285765	-1.471759	-2.054942
	1	2.677563	-2.319476	-1.464899
	1	2.637541	-1.564951	-3.100388
	1	2.673482	-0.537545	-1.612924
	6	0.000000	-2.905698	-3.003909
	1	0.474460	-2.844281	-4.001538
	1	0.333045	-3.834087	-2.506381
	1	-1.096583	-2.957760	-3.118056
	6	0.000000	-2.905698	3.003909
	1	0.333045	-3.834087	2.506381
	1	0.474460	-2.844281	4.001538
	1	-1.096583	-2.957760	3.118056
	6	2.285765	-1.471759	2.054942
	1	2.637541	-1.564951	3.100388
	1	2.677563	-2.319476	1.464899
	1	2.673482	-0.537545	1.612924
	6	0.000000	0.000000	3.036414
	1	0.853983	0.270537	3.686233
	1	-0.853983	-0.270537	3.686233
	6	-2.285765	1.471759	2.054942
	1	-2.637541	1.564951	3.100388
	1	-2.677563	2.319476	1.464899
	1	-2.673482	0.537545	1.612924
	6	0.000000	2.905698	3.003909
	1	-0.333045	3.834087	2.506381
	1	-0.474460	2.844281	4.001538
	1	1.096583	2.957760	3.118056
	28	1.271868	-0.064877	0.000000
	28	-1.165926	-0.102541	0.000000
	15	1.595896	-0.024636	2.204411
	15	-1.657328	-0.020589	2.144456
	15	1.595896	-0.024636	-2.204411
	15	-1.657328	-0.020589	-2.144456
$[(Me_2P)_2CH_2]_2Ni_2(CO)_2$	6	-0.059796	-1.593437	0.000000
S-PMe-22-3S(*C*$_S$)	8	0.298988	-2.736298	0.000000
	6	-0.037784	1.382143	0.000000
	8	0.195000	2.562160	0.000000
	6	-2.828440	-1.163334	-3.033252
	1	-3.862165	-0.908722	-2.738039
	1	-2.740732	-1.095621	-4.134421

	1	-2.630289	-2.201226	-2.713156
	6	-2.086852	1.599734	-2.949406
	1	-2.040587	1.550200	-4.053890
	1	-3.108167	1.888165	-2.643265
	1	-1.395642	2.379713	-2.586115
	6	-0.046649	-0.478287	-3.032358
	1	-0.055694	-0.113736	-4.079505
	1	-0.049163	-1.585449	-3.070638
	6	1.979136	1.622901	-2.971675
	1	3.019298	1.898025	-2.723004
	1	1.860510	1.604556	-4.071379
	1	1.315235	2.391785	-2.541321
	6	2.734898	-1.138108	-3.167362
	1	2.583853	-1.055201	-4.260654
	1	3.779451	-0.873621	-2.924484
	1	2.566609	-2.183627	-2.854965
	6	-2.086852	1.599734	2.949406
	1	-3.108167	1.888165	2.643265
	1	-2.040587	1.550200	4.053890
	1	-1.395642	2.379713	2.586115
	6	-0.046649	-0.478287	3.032358
	1	-0.049163	-1.585449	3.070638
	1	-0.055694	-0.113736	4.079505
	6	2.734898	-1.138108	3.167362
	1	3.779451	-0.873621	2.924484
	1	2.583853	-1.055201	4.260654
	1	2.566609	-2.183627	2.854965
	6	1.979136	1.622901	2.971675
	1	1.860510	1.604556	4.071379
	1	3.019298	1.898025	2.723004
	1	1.315235	2.391785	2.541321
	6	-2.828440	-1.163334	3.033252
	1	-2.740732	-1.095621	4.134421
	1	-3.862165	-0.908722	2.738039
	1	-2.630289	-2.201226	2.713156
	28	-0.108105	-1.325602	0.134062
	28	0.084580	1.121960	0.721009
$[(Me_2P)_2CH_2]_2Ni_2(CO)_2$	6	-0.219427	-3.056807	0.538439
	8	-0.294144	-4.205521	0.818423
S-PMe-22-1T(C_1)	15	-2.187132	-0.986987	-0.583822
	15	-1.710490	2.007981	-0.173535
	15	1.964189	-1.285593	-0.682743

15	2.065711	1.706276	-0.027132
6	-0.073692	-0.085566	2.042933
8	-0.176323	-0.647038	3.101864
6	-2.582756	0.720017	-1.224303
1	-2.139407	0.778112	-2.237275
1	-3.674458	0.894492	-1.314506
6	-3.077146	2.575177	0.961087
1	-2.702912	3.420332	1.565853
1	-3.980276	2.898185	0.408453
1	-3.342412	1.761510	1.657111
6	-3.444089	-1.230548	0.756694
1	-4.463932	-0.955438	0.428332
1	-3.432639	-2.291992	1.060820
1	-3.156844	-0.631077	1.636933
6	-2.893739	-2.061506	-1.929227
1	-2.816177	-3.117164	-1.614633
1	-3.952818	-1.826138	-2.146832
1	-2.296921	-1.936915	-2.849793
6	-1.687191	3.453354	-1.351236
1	-2.691583	3.685335	-1.753693
1	-1.302835	4.342809	-0.820638
1	-1.003034	3.233552	-2.189786
6	2.391367	3.228766	-1.053052
1	2.200146	4.125746	-0.437126
1	3.431926	3.269783	-1.427158
1	1.696297	3.249650	-1.910695
6	3.482280	1.850794	1.175687
1	4.456030	1.997233	0.670126
1	3.289621	2.709959	1.842728
1	3.526537	0.946676	1.806066
6	2.670541	0.366159	-1.192180
1	3.774664	0.335225	-1.296881
1	2.236263	0.594349	-2.184984
6	3.202791	-1.896546	0.554976
1	2.989124	-2.957867	0.772082
1	4.242417	-1.799918	0.189894
1	3.082622	-1.334753	1.496544
6	2.404128	-2.334070	-2.158153
1	3.478712	-2.269561	-2.414488
1	2.148235	-3.384578	-1.934061
1	1.803490	-2.015609	-3.028185

Complete Gaussian 09 reference (Reference 26)

Gaussian 09, Revision D.01,

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