The Remarkable $Nb_2(CO)_{12}$ with Seven-Coordinate Niobium: Decarbonylation to $Nb_2(CO)_{11}$ and $Nb_2(CO)_{10}$

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Supporting Information

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Tables S5–S8. Harmonic vibrational frequencies and infrared intensities for four singlet structures of $Nb_2(CO)_{11}$.
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Table S21 Cartesian coordinates of **12S-1,12S-2,12S-3,12S-4**

Table S22 Cartesian coordinates of **11S-1,11S-2,11S-3,11S-4**

Table S23 Cartesian coordinates of **11T-1,11T-2,11T-3**

Table S24 Cartesian coordinates of **10S-1,10S-2,10S-3,10S-4,10S-5**

Table S25 Cartesian coordinates of **10T-1,10T-2,10T-3,10T-4**

Table S26. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **6D-1** of doublet Nb $(CO)_6$ with D_{3d} symmetry. The IR intensities are doubled for the doubly degenerate modes.

Table 27. Cartesian coordinates of **16S-1**.

Table S1. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, km/mol) for structure **12S-1** of singlet $Nb_2(CO)_{12}$ with C_2 symmetry.

	MPW1PW91		BP86			MPW1PW91		BP86	
a	27	(3)	25	(2)	b	32	(0)	29	(0)
	36	(0)	34	(0)		44	(0)	37	(0)
	60	(0)	57	(0)		51	(0)	47	(0)
	77	(0)	71	(0)		65	(0)	60	(0)
	80	(0)	72	(0)		69	(0)	63	(0)
	83	(0)	78	(0)		81	(0)	76	(1)
	85	(2)	79	(2)		85	(1)	79	(1)
	92	(1)	87	(1)		86	(0)	81	(0)
	89	(0)	96	(0)		91	(0)	85	(0)
	101	(0)	94	(0)		95	(0)	90	(0)
	109	(0)	103	(0)		101	(0)	92	(0)
	120	(0)	111	(0)		109	(0)	104	(0)
	308	(39)	297	(40)		353	(12)	342	(3)
	334	(1)	313	(0)		360	(3)	345	(1)
	347	(0)	334	(0)		365	(4)	361	(6)
	350	(2)	338	(1)		372	(19)	363	(0)
	360	(1)	350	(2)		375	(2)	364	(1)
	374	(2)	363	(3)		384	(8)	365	(3)
	394	(2)	385	(5)		388	(1)	371	(9)
	415	(21)	406	(13)		398	(27)	391	(16)
	420	(0)	408	(0)		414	(24)	405	(18)
	466	(0)	441	(6)		422	(6)	411	(0)
	470	(2)	446	(2)		438	(7)	415	(6)
	491	(4)	463	(1)		467	(7)	443	(0)
	507	(9)	479	(6)		503	(4)	476	(4)
	511	(20)	486	(13)		519	(8)	490	(7)
	524	(157)	502	(49)		552	(24)	525	(15)
	546	(70)	518	(127)		555	(67)	531	(55)
	561	(73)	533	(45)		561	(40)	534	(27)
	564	(83)	539	(31)		564	(46)	541	(70)
	2056	(401)	1937	(307)		2063	(522)	1944	(374)
	2067	(489)	1945	(300)		2079	(1248)	1959	(574)
	2081	(873)	1960	(714)		2084	(386)	1963	(419)
	2094	(192)	1973	(185)		2110	(1839)	1983	(1783)
	2112	(44)	1984	(38)		2118	(2780)	1990	(2432)
	2141	(1917)	2019	(1730)		2198	(5)	2067	(5)

Table S2. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, km/mol) for structure **12S-2** of singlet $Nb_2(CO)_{12}$ with D_2 symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86		MPW1PW91	BP86
A	35(0)	29(0)	B1	17i	17i	B3	34(0)	30(0)
	57(0)	56(0)		82(1)	76(1)		62(0)	59(0)
	78(0)	71(0)		83(0)	78(0)		81(2)	76(2)
	83(0)	74(0)		93(2)	86(3)		85(0)	80(0)
	96(0)	86(0)		99(1)	93(1)		92(0)	87(0)
	106(0)	100(0)		296(68)	281(70)		105(0)	100(0)
	120(0)	110(0)		350(2)	336(4)		359(8)	348(1)
	323(0)	308(0)		361(2)	354(1)		372(14)	355(9)
	350(0)	336(0)		382(5)	354(1)		382(1)	364(1)
	360(0)	352(0)		418(8)	375(8)		397(11)	414(29)
	377(0)	371(0)		470(2)	411(7)		462(5)	389(3)
	420(0)	411(0)		498(24)	447(3)		512(12)	401(20)
	467(0)	443(0)		525(34)	467(7)		555(3)	432(6)
	502(0)	469(0)		541(285)	496(1)		556(103)	483(9)
	527(0)	496(0)		2075(1217)	1955(842)		2070(179)	1949(1)
	557(0)	536(0)		2093(387)	1970(0)		2081(1260)	1960(0)
	2093(0)	1969(416)		2141(1851)	2019(1709)		2102(2324)	
1977(2169)								
	2096(0)	1972(0)						
	2196(0)	2065(0)						
B2	45(0)	31(0)						
	58(0)	52(0)						
	69(0)	63(0)						
	85(3)	78(2)						
	96(0)	88(0)						
	102(0)	91(0)						
	361(10)	345(0)						
	370(8)	354(12)						
	362(3)	380(10)						
	387(12)	402(6)						
	389(9)	411(8)						
	414(9)	484(2)						
	437(8)	530(39)						
	513(4)	535(13)						
	557(59)	527(4)						
	559(11)	532(76)						
	2065(33)	1945(13)						
	2083(51)	1961(891)						
	2112(3278)	1985(2817)						

Table S3. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, km/mol) for structure **12S-3** of singlet $Nb_2(CO)_{12}$ with D_{3d} symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86		MPW1PW91	BP86
A	65(0)	61(0)	A1G	62(0)	57(0)	A1U	43(0)	39(0)
	70(0)	64(0)		95(0)	85(0)		351(0)	335(0)
	70(0)	64(0)		116(0)	109(0)		510(0)	488(0)
B	83(3)	75(0)		359(0)	349(0)	A2U	75(2)	72(1)
	83(3)	77(2)		390(0)	385(0)		99(1)	92(1)
	84(0)	78(0)		453(0)	432(0)		347(4)	333(0)
EG	32(0)	31(0)		545(0)	514(0)		384(71)	376(41)
	32(0)	31(0)		2085(0)	1961(0)		447(3)	426(7)
	84(0)	77(2)		2200(0)	2069(0)		523(397)	498(312)
	84(0)	78(0)	A2G	351(0)	338(1)		2065(514)	1945(703)
	98(0)	90(0)		507(0)	486(0)		2140(4113)	
2019(3122)								
	98(0)	90(0)						
	322(0)	310(0)						
	322(0)	310(0)						
	355(0)	348(0)						
	355(0)	349(0)						
	385(0)	376(41)						
	385(0)	382(45)						
	432(0)	413(0)						
	432(0)	413(0)						
	466(0)	443(0)						
	466(0)	443(0)						
	569(0)	542(0)						
	569(0)	542(0)						
	2052(0)	1937(0)						
	2052(0)	1937(0)						
	2105(0)	1977(0)						
	2105(0)	1977(0)						

Table S4. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, km/mol) for structure **12S-4** of singlet $Nb_2(CO)_{12}$ with C_{2v} symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86		MPW1PW91	BP86
A1	38(0)	37(0)	A2	200i	145i	B1	11i	4(0)
	65(0)	63(0)		17i	13i		74(2)	69(1)
	78(2)	74(1)		62(0)	58(0)		81(0)	75(0)
	85(1)	81(1)		77(0)	74(0)		93(1)	78(0)
	113(0)	106(0)		94(0)	89(0)		102(1)	88(1)
	118(0)	111(0)		108(0)	104(0)		259(4)	97(0)
	145(0)	137(0)		218(0)	211(0)		346(0)	246(3)
	291(1)	280(1)		343(0)	329(0)		371(24)	333(0)
	358(1)	349(1)		378(0)	369(0)		379(19)	359(3)
	369(11)	358(12)		421(0)	401(0)		456(21)	372(19)
	375(49)	370(20)		485(0)	463(0)		473(11)	428(13)
	385(4)	372(10)		504(0)	479(0)		509(0)	451(14)
	429(17)	414(15)		498(23)	478(47)		556(88)	484(0)
	446(3)	433(0)		561(0)	535(0)		1929(711)	1829(402)
	462(0)	441(0)		2095(0)	1968(0)		2107(3280)	1981(2715)
	512(0)	488(0)						
	559(60)	531(45)						
	575(8)	548(5)						
	1945(179)	1836(118)						
	2084(5)	1962(19)						
	2100(3583)	1973(13)						
	2113(4)	1983(171)						
	2197(21)	2064(15)						
B2	53(0)	52(1)						
	57(2)	54(0)						
	79(1)	87(0)						
	90(1)	94(0)						
	99(0)	214(12)						
	226(13)	344(10)						
	353(15)	351(1)						
	361(0)	368(7)						
	379(5)	381(11)						
	385(18)	387(25)						
	405(27)	418(12)						
	422(40)	478(47)						
	498(23)	492(136)						
	523(186)	527(2)						
	560(6)	531(63)						
	569(250)	540(169)						
	2065(461)	1946(246)						
	2079(1626)	1959(1208)						
	2102(6)	1977(2761)						
	2143(2476)	2019(2226)						

Table S5. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **11S-1** of singlet $Nb_2(CO)_{11}$ with C_1 symmetry.

	MPW1PW91		BP86	
A	20(0)	389(13)	22(0)	377(1)
	27(0)	391(21)	22(0)	381(3)
	36(0)	396(6)	34(0)	382(19)
	46(0)	409(10)	42(0)	397(7)
	54(0)	422(4)	49(0)	404(4)
	61(0)	431(9)	56(0)	417(8)
	67(0)	437(13)	63(0)	423(18)
	69(0)	440(12)	64(0)	425(5)
	71(0)	453(2)	65(0)	432(0)
	73(0)	458(0)	69(0)	433(1)
	74(0)	474(33)	69(0)	56(24)
	75(0)	481(9)	71(0)	462(5)
	80(0)	506(7)	76(0)	485(3)
	83(0)	518(5)	78(0)	493(3)
	85(0)	529(17)	79(0)	502(6)
	91(0)	530(49)	85(0)	508(17)
	94(1)	546(10)	87(1)	513(24)
	98(0)	552(36)	89(0)	528(27)
	110(1)	558(19)	104(1)	532(25)
	115(0)	562(116)	109(0)	535(80)
	126(1)	578(41)	119(1)	547(30)
	256(17)	623(117)	245(9)	584(108)
	317(8)	1795(751)	312(3)	1701(523)
	323(12)	2055(333)	319(8)	1939(188)
	338(2)	2069(289)	321(4)	1952(413)
	341(3)	2071(1273)	327(3)	1953(454)
	346(27)	2091(345)	338(26)	1968(542)
	349(7)	2093(2175)	346(6)	1970(1445)
	359(7)	2100(693)	350(3)	1972(754)
	364(3)	2116(2651)	352(11)	1984(2544)
	378(7)	2121(115)	364(3)	1986(230)
	378(5)	2152(2116)	367(6)	2024(1822)
	386(30)	2195(30)	376(25)	2063(27)

Table S6. Harmonic vibrational frequencies (cm-1) and infrared intensities (in patentheses, in km/mol) for structre **11S-2** of singlet Nb2(CO)11 with Cs symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
a'	37(0)	29(0)	a"	22i	20i
	48(1)	47(0)		20(0)	6i
	69(0)	66(0)		32(1)	30(0)
	76(0)	71(0)		51(0)	47(0)
	81(2)	76(1)		62(0)	59(0)
	85(0)	79(1)		67(0)	64(0)
	88(2)	81(0)		85(2)	78(1)
	92(0)	87(0)		87(0)	83(0)
	98(0)	93(0)		97(0)	87(0)
	119(1)	122(2)		111(0)	112(0)
	130(1)	130(1)		319(10)	294(11)
	149(0)	141(0)		334(5)	317(6)
	336(2)	324(0)		349(0)	327(2)
	342(16)	328(3)		352(0)	330(0)
	349(26)	342(19)		361(18)	340(1)
	367(0)	357(10)		375(0)	363(0)
	372(14)	358(9)		387(1)	370(1)
	386(2)	374(1)		394(23)	385(20)
	401(3)	396(13)		406(23)	395(15)
	418(10)	407(0)		448(0)	426(0)
	445(70)	432(37)		460(7)	439(1)
	456(2)	441(25)		469(0)	452(4)
	484(1)	463(1)		504(1)	474(0)
	502(50)	477(66)		549(18)	519(5)
	522(116)	488(59)		560(49)	533(46)
	536(9)	501(10)		2033(496)	1912(51)
	537(9)	507(16)		2073(1689)	1943(1431)
	547(19)	518(17)		2090(951)	1966(989)
	559(41)	533(24)		2138(593)	2002(565)
	595(53)	565(36)			
	1982(397)	1877(269)			
	2061(607)	1930(499)			
	2069(859)	1949(503)			
	2095(353)	1967(461)			
	2113(1923)	1985(1569)			
	2136(2892)	2009(2588)			
	2195(127)	2060(127)			

Table S7. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **11S-3** of singlet $Nb_2(CO)_{11}$ with C_2 symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
a	36(0)	34(0)	b	384i	355i
	39(0)	36(0)		90i	107i
	61(0)	57(0)		44(0)	41(0)
	66(0)	62(0)		46(0)	46(1)
	69(2)	64(1)		60(0)	56(0)
	72(0)	69(0)		72(0)	69(0)
	80(1)	76(0)		78(6)	72(6)
	85(0)	81(0)		84(2)	79(1)
	92(0)	86(0)		88(0)	84(0)
	112(0)	104(0)		92(1)	86(0)
	147(0)	137(0)		110(2)	103(3)
	279(1)	278(0)		181(0)	179(0)
	331(3)	321(1)		312(18)	285(2)
	348(0)	338(1)		327(17)	316(16)
	360(0)	347(0)		343(3)	332(4)
	365(0)	357(0)		351(20)	339(14)
	375(1)	362(4)		362(0)	356(5)
	386(11)	376(8)		373(13)	361(21)
	415(1)	399(1)		385(88)	374(61)
	418(0)	408(0)		394(12)	379(6)
	440(6)	426(3)		423(40)	411(18)
	482(13)	454(8)		436(29)	418(36)
	501(1)	478(0)		471(59)	446(32)
	523(26)	496(11)		498(4)	474(1)
	525(8)	497(14)		513(1)	483(0)
	554(5)	524(4)		524(37)	494(38)
	573(10)	1896(261)		537(53)	509(32)
	2043(173)	1937(14)		559(117)	534(92)
	2053(15)	1953(445)		2038(74)	1926(103)
	2074(1685)	1959(1306)		2062(535)	1946(262)
	2079(656)	1975(661)		2092(1664)	1966(1117)
	2105(813)	1976(2155)		2103(2489)	1976(2155)
	2191(2)	2058(0)		2123(3852)	2001(3328)

Table S8. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **11S-4** of singlet $Nb_2(CO)_{11}$ with C_s symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
A'	32(0)	26(0)	A"	18(0)	14(0)
	45(0)	38(0)		35(0)	30(0)
	68(0)	62(0)		42(1)	36(1)
	72(0)	67(0)		67(0)	60(0)
	75(1)	69(1)		68(0)	65(0)
	85(0)	78(0)		85(1)	81(1)
	92(1)	88(0)		87(0)	82(0)
	94(1)	89(0)		91(0)	85(0)
	101(0)	94(0)		96(0)	89(0)
	113(0)	108(0)		102(0)	98(0)
	117(0)	111(0)		339(0)	327(0)
	132(0)	123(0)		341(8)	327(0)
	279(7)	263(0)		345(0)	334(0)
	341(8)	336(1)		349(0)	337(0)
	345(8)	339(8)		357(15)	354(11)
	356(11)	351(13)		383(3)	359(2)
	361(32)	355(20)		388(30)	373(1)
	384(0)	367(9)		392(15)	379(29)
	395(3)	385(4)		467(0)	441(0)
	414(21)	406(9)		499(8)	478(7)
	421(0)	412(3)		511(5)	483(7)
	437(7)	421(6)		517(12)	488(3)
	453(6)	438(0)		520(140)	498(1)
	468(0)	445(1)		552(26)	524(17)
	485(25)	468(19)		2026(1321)	1913(1025)
	520(140)	497(1)		2124(1354)	1993(1191)
	527(0)	499(92)		2133(822)	1999(754)
	539(12)	513(24)			
	550(23)	523(13)			
	552(26)	523(17)			
	554(26)	529(24)			
	557(41)	533(42)			
	594(74)	567(49)			
	1981(624)	1877(783)			
	2020(589)	1883(103)			
	2072(403)	1947(389)			
	2076(1048)	1958(633)			
	2093(774)	1974(588)			
	2119(1481)	1991(957)			
	2124(1354)	1992(1191)			
	2127(1695)	1999(1912)			
	2198(67)	2066(84)			

Table S9. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **11T-1** of triplet $Nb_2(CO)_{11}$ with C_s symmetry.

	MPW1PW91	BP86
A'	33(0)	34(0)
	50(0)	48(0)
	58(0)	55(0)
	63(0)	59(0)
	69(0)	67(0)
	72(0)	68(0)
	78(0)	74(0)
	81(0)	76(0)
	95(0)	89(0)
	107(0)	101(0)
	118(1)	115(0)
	169(0)	175(0)
	310(1)	278(0)
	339(0)	322(1)
	347(0)	343(0)
	354(20)	346(9)
	359(4)	352(5)
	363(6)	355(4)
	363(45)	359(0)
	386(91)	384(53)
	390(9)	386(10)
	404(25)	396(9)
	425(0)	404(5)
	440(3)	420(4)
	453(0)	431(0)
	471(9)	445(0)
	473(0)	457(6)
	505(67)	487(67)
	542(75)	510(28)
	547(54)	522(61)
	558(30)	529(11)
	1961(417)	1843(262)
	2051(13)	1936(98)
	2085(524)	1961(536)
	2086(2606)	1965(1250)
	2097(10)	1972(772)
	2105(628)	1976(538)
	2125(4546)	2004(3642)
	2195(7)	2062(17)

	MPW1PW91	BP86
A"	15i	11i
	25(0)	26(0)
	40(0)	37(0)
	54(0)	54(0)
	61(0)	59(0)
	66(0)	60(0)
	77(0)	73(0)
	77(0)	73(0)
	79(0)	75(0)
	101(0)	92(0)
	332(1)	316(0)
	334(0)	319(0)
	340(2)	325(0)
	346(6)	331(0)
	361(0)	353(2)
	367(3)	361(32)
	383(20)	371(8)
	416(0)	402(0)
	441(0)	423(0)
	450(4)	428(0)
	464(1)	438(1)
	491(0)	463(0)
	523(40)	499(24)
	546(40)	515(44)
	2059(132)	1942(3)
	2098(3443)	1972(2824)
	1210(380)	1974(94)

Table S10. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **11T-2** of triplet $Nb_2(CO)_{11}$ with C_2 symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
A	27(0)	25(0)	B	165i	101i
	43(0)	40(0)		3(0)	12(0)
	57(0)	54(0)		33(0)	34(0)
	59(0)	58(0)		53(0)	50(0)
	64(0)	60(0)		60(0)	57(0)
	71(0)	66(0)		73(0)	69(0)
	74(0)	69(0)		76(0)	74(0)
	80(0)	76(0)		79(0)	75(0)
	88(0)	82(0)		85(0)	84(0)
	114(0)	105(0)		94(0)	89(0)
	142(0)	131(0)		108(0)	110(3)
	307(1)	296(0)		230(0)	220(0)
	344(0)	318(0)		334(28)	318(0)
	354(1)	333(0)		340(0)	324(0)
	358(16)	350(1)		345(4)	340(1)
	366(8)	353(8)		354(5)	348(9)
	377(3)	356(1)		359(5)	355(1)
	396(0)	368(7)		371(52)	365(32)
	418(20)	392(0)		387(100)	385(57)
	430(0)	403(15)		418(1)	404(1)
	445(0)	412(0)		425(1)	408(0)
	466(0)	423(0)		442(2)	419(1)
	488(0)	447(0)		458(4)	431(3)
	525(25)	467(0)		473(1)	453(2)
	532(10)	499(13)		488(3)	462(0)
	532(85)	508(3)		506(100)	487(96)
	549(63)	521(52)		532(85)	507(59)
	1936(282)	1831(212)		550(29)	522(21)
	2061(112)	1943(19)		2048(20)	1935(56)
	2086(1672)	1966(980)		2093(262)	1966(389)
	2096(578)	1969(653)		2096(259)	1971(45)
	2103(1189)	1975(971)		2099(3144)	1973(2878)
	2194(2)	2062(3)		2122(4912)	2003(2672)

Table S11. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **11T-3** of triplet $Nb_2(CO)_{11}$ with C_{2v} symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
A1	54(0)	51(0)	B1	10i	25i
	66(0)	62(0)		56(0)	53(0)
	77(0)	73(0)		62(0)	59(0)
	81(0)	77(0)		74(0)	69(0)
	117(0)	108(0)		81(0)	76(0)
	150(0)	142(0)		92(0)	84(0)
	339(0)	325(0)		331(0)	311(0)
	359(18)	357(1)		347(1)	332(0)
	363(1)	358(0)		368(30)	361(19)
	382(68)	380(31)		369(46)	365(32)
	391(15)	388(7)		433(2)	407(0)
	449(19)	430(10)		457(0)	432(0)
	455(7)	434(3)		537(0)	507(16)
	483(12)	457(17)		548(85)	519(46)
	502(78)	479(51)		2069(27)	1948(8)
	525(13)	504(42)		2099(3653)	1973(3012)
	2021(0)	1900(66)	B2	43i	58i
	2087(1583)	1964(834)		23(0)	17i
	2097(216)	1976(10)		51(0)	47(0)
	2126(3948)	2009(3017)		69(0)	65(0)
	2195(8)	2062(7)		73(1)	68(1)
A2	26(0)	23(0)		133(0)	124(0)
	41(0)	36(0)		308(0)	279(1)
	65(0)	62(0)		338(3)	321(0)
	87(0)	82(0)		349(22)	348(13)
	337(0)	321(0)		364(12)	351(4)
	340(0)	323(0)		371(0)	359(8)
	353(0)	349(0)		413(21)	401(13)
	439(0)	420(0)		486(0)	462(0)
	449(0)	426(0)		541(60)	513(40)
	474(0)	450(0)		568(36)	542(25)
	2093(0)	1968(0)		2007(593)	1890(396)
				2089(1766)	1963(1333)
				2106(1219)	1978(1113)

Table S12. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, km/mol) for structure **10S-1** of singlet $Nb_2(CO)_{10}$ with C_s symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
A'	39(0)	38(0)	A"	4(0)	2(0)
	61(0)	60(0)		39(0)	38(0)
	69(0)	66(0)		52(0)	46(0)
	70(0)	67(0)		61(0)	59(0)
	84(1)	79(0)		68(0)	66(0)
	90(0)	87(0)		78(0)	76(0)
	97(0)	93(0)		87(0)	83(0)
	102(0)	96(0)		98(0)	93(0)
	130(0)	124(0)		129(0)	123(0)
	141(0)	136(0)		327(0)	311(0)
	173(0)	167(0)		347(0)	329(0)
	328(0)	312(0)		358(15)	353(8)
	358(18)	355(6)		369(3)	362(3)
	368(14)	355(7)		405(16)	390(8)
	378(37)	375(31)		408(2)	394(2)
	404(15)	387(9)		417(1)	403(0)
	412(0)	399(0)		447(28)	432(4)
	416(1)	401(0)		456(4)	447(13)
	447(32)	433(5)		479(0)	458(2)
	452(1)	435(5)		484(2)	460(0)
	458(1)	447(13)		488(2)	465(5)
	487(7)	463(10)		539(9)	511(7)
	540(10)	512(8)		568(46)	542(34)
	565(97)	537(162)		2015(698)	1900(514)
	565(156)	538(28)		2069(1935)	1950(733)
	573(0)	540(10)		2078(160)	1952(881)
	581(4)	554(2)		2122(791)	1992(714)
	2014(640)	1900(464)			
	2038(500)	1916(373)			
	2070(2087)	1951(1612)			
	2122(814)	1992(736)			
	2141(2255)	2015(1901)			
	2184(304)	2053(285)			

Table S13. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, km/mol) for structure **10S-2** of singlet $Nb_2(CO)_{11}$ with C_{2v} symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
A1	61(0)	56(0)	A2	9(0)	7(0)
	70(0)	67(0)		40(0)	37(0)
	93(0)	89(0)		71(0)	68(0)
	103(0)	97(0)		80(0)	78(0)
	147(0)	140(0)		341(0)	323(0)
	164(4)	59(2)		367(0)	359(0)
	354(17)	343(7)		414(0)	402(0)
	371(2)	363(0)		450(0)	428(0)
	380(29)	376(21)		470(0)	450(0)
	410(0)	398(3)		499(0)	479(0)
	462(10)	440(19)		2076(0)	1949(0)
	476(7)	56(6)			
	553(170)	525(128)			
	576(1)	543(1)			
	583(7)	557(6)			
	2010(526)	1885(404)			
	2107(98)	1982(113)			
	2142(2137)	2017(1686)			
	2182(275)	2051(286)			
B1	54i	53i	B2	40(0)	38(0)
	42(0)	41(0)		55(0)	51(0)
	72(0)	69(0)		87(1)	82(0)
	80(1)	75(0)		100(0)	94(0)
	100(0)	95(0)		160(0)	155(0)
	321(2)	304(0)		307(5)	280(3)
	384(28)	371(19)		355(22)	352(12)
	412(0)	394(0)		383(18)	368(9)
	438(0)	413(0)		407(13)	393(7)
	450(37)	450(26)		447(32)	443(24)
	543(13)	515(5)		480(2)	459(0)
	553(45)	526(35)		529(5)	500(3)
	2065(283)	1947(287)		566(53)	540(38)
	2087(3079)	1967(2471)		1995(1052)	1877(756)
				2065(1989)	1946(1481)
				2120(807)	1991(724)

Table S14. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (km/mol, in parentheses) for structure **10S-3** of singlet $Nb_2(CO)_{10}$ with C_2 symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
A	17(0)	15(0)	B	12i	20i
	29(0)	25(0)		45(0)	42(0)
	53(0)	51(0)		54(0)	54(0)
	63(0)	61(0)		61(0)	58(0)
	65(0)	63(0)		68(0)	65(0)
	71(1)	68(1)		78(0)	75(0)
	77(0)	74(0)		82(1)	84(0)
	90(0)	79(0)		88(0)	151(0)
	98(0)	84(0)		157(1)	298(10)
	164(0)	94(0)		319(9)	325(6)
	190(0)	159(0)		339(8)	333(2)
	317(0)	175(0)		346(4)	351(6)
	335(10)	306(0)		354(31)	354(9)
	354(0)	325(3)		360(25)	366(28)
	359(11)	338(1)		373(15)	400(55)
	370(0)	354(8)		411(1)	402(1)
	378(10)	361(1)		415(65)	416(7)
	401(30)	372(3)		428(20)	434(2)
	407(1)	388(23)		458(3)	455(1)
	438(0)	398(0)		475(3)	481(19)
	443(1)	418(0)		502(28)	492(32)
	477(0)	424(0)		512(76)	499(49)
	497(4)	458(0)		522(32)	530(83)
	524(31)	475(3)		557(101)	1890(804)
	539(15)	499(26)		2006(1166)	1957(53)
	565(2)	519(6)		2081(250)	1964(2275)
	1986(76)	533(2)		2085(2755)	1978(157)
	2082(10)	1874(57)		2112(180)	1979(1535)
	2109(3254)	1960(3)		2139(3149)	2012(2669)
	2116(75)	1983(1189)			
	2193(1)	2058(4)			

Table S15. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (km/mol, in parentheses) for structure **10S-4** of singlet $Nb_2(CO)_{10}$ with C_{2h} symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
AG	52(0)	47(0)	AU	17i	22i
	55(0)	52(0)		25(0)	18(0)
	72(0)	69(0)		61(1)	59(1)
	103(0)	98(0)		71(0)	69(0)
	167(0)	159(0)		79(1)	75(1)
	193(0)	179(0)		327(7)	314(2)
	326(0)	319(0)		348(4)	333(1)
	361(0)	355(0)		384(53)	375(37)
	368(0)	364(0)		427(0)	406(0)
	385(0)	370(0)		473(1)	456(0)
	411(0)	400(0)		518(51)	490(38)
	436(0)	417(0)		2113(3461)	1985(2855)
	497(0)	477(0)	BU	41(0)	35(0)
	535(0)	516(0)		53(2)	50(1)
	574(0)	542(0)		64(0)	60(0)
	1981(0)	1867(0)		83(1)	80(0)
	2078(0)	1957(0)		160(1)	153(1)
	2122(0)	1987(0)		331(21)	309(15)
	2195(0)	2060(0)		348(46)	347(26)
BG	34(0)	29(0)		361(22)	353(3)
	55(0)	50(0)		372(4)	361(17)
	77(0)	74(0)		419(63)	403(83)
	89(0)	85(0)		428(44)	416(6)
	333(0)	321(0)		498(49)	478(34)
	343(0)	328(0)		514(73)	496(48)
	394(0)	384(0)		561(103)	534(89)
	456(0)	433(0)		2005(1188)	1888(840)
	474(0)	454(0)		2080(2802)	1960(2119
	514(0)	489(0)		2111(334)	1979(318)
	2091(0)	1966(0)		2139(3116)	2013(2618)

Table S16. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (km/mol, in parentheses) for structure **10S-5** of singlet $Nb_2(CO)_{10}$ with C_2 symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
A	22(0)	26(0)	B	22(0)	18(0)
	53(0)	50(0)		34(0)	33(0)
	58(0)	58(0)		57(0)	55(0)
	66(0)	63(0)		64(0)	61(0)
	67(0)	65(0)		69(0)	66(0)
	78(1)	75(1)		75(0)	72(0)
	85(0)	81(0)		86(0)	83(0)
	104(0)	101(0)		87(0)	84(0)
	122(1)	119(1)		122(0)	120(0)
	227(24)	218(10)		214(2)	209(1)
	331(5)	316(5)		320(3)	312(1)
	342(22)	335(4)		336(2)	320(0)
	348(8)	347(12)		347(22)	343(15)
	379(2)	370(2)		349(27)	345(19)
	381(0)	371(1)		378(9)	363(0)
	395(6)	381(4)		384(25)	373(24)
	413(0)	403(2)		393(1)	381(0)
	432(12)	415(0)		405(30)	405(18)
	436(0)	424(8)		438(6)	416(3)
	446(11)	432(9)		452(6)	427(4)
	497(13)	469(18)		501(3)	476(3)
	524(10)	503(8)		534(23)	506(14)
	535(33)	513(18)		548(28)	523(20)
	566(6)	542(1)		568(56)	539(37)
	603(101)	568(80)		586(62)	559(45)
	1869(664)	1754(430)		1834(920)	1729(650)
	2066(823)	1942(563)		2054(65)	1934(234)
	2106(137)	1979(217)		2070(832)	1943(543)
	2145(2263)	2015(1976)		2090(3582)	1967(2851)
	2185(208)	2052(188)		2132(824)	1995(779)

Table S17. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (km/mol, in parentheses) for structure **10T-1** of triplet $Nb_2(CO)_{10}$ with C_1 symmetry.

	MPW1PW91	BP86	MPW1PW91	BP86
A	11(0)	13(0)	372(42)	363(42)
	24(0)	21(0)	376(39)	366(0)
	36(0)	33(0)	385(12)	373(35)
	40(0)	40(0)	389(20)	384(7)
	41(0)	44(0)	408(14)	391(2)
	53(0)	50(0)	413(9)	403(4)
	58(0)	55(0)	426(3)	412(7)
	60(0)	58(0)	436(3)	416(0)
	66(0)	61(0)	441(0)	420(0)
	67(0)	62(0)	447(0)	423(2)
	70(0)	67(0)	457(0)	433(1)
	71(0)	68(0)	460(9)	448(5)
	73(0)	71(0)	480(7)	458(4)
	78(1)	76(0)	484(38)	465(35)
	80(0)	77(0)	509(18)	484(14)
	83(0)	82(0)	518(25)	500(10)
	101(0)	99(0)	540(30)	508(18)
	115(0)	109(0)	542(66)	509(42)
	140(0)	146(0)	559(44)	528(34)
	176(2)	169(0)	608(56)	575(39)
	317(1)	277(6)	1875(545)	1773(368)
	325(0)	309(0)	2009(265)	1878(235)
	338(0)	323(0)	2057(38)	1935(205)
	339(11)	328(0)	2065(1372)	1943(687)
	340(12)	330(0)	2079(251)	1947(481)
	348(1)	336(12)	2091(3522)	1969(2672)
	356(12)	344(5)	2099(466)	1976(36)
	357(3)	350(7)	2118(1788)	1987(863)
	364(6)	353(3)	2128(3132)	1998(3499)
	365(28)	360(0)	2187(111)	2054(138)

Table S18. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (km/mol, in parentheses) for structure **10T-2** of triplet $Nb_2(CO)_{10}$ with C_1 symmetry.

	MPW1PW91	BP86	MPW1PW91	BP86
A	16(0)	12(0)	369(18)	362(21)
	21(0)	24(0)	371(26)	363(25)
	43(0)	40(0)	373(17)	365(2)
	45(0)	43(0)	399(2)	390(4)
	50(0)	46(0)	408(42)	400(15)
	53(0)	51(0)	414(0)	407(0)
	54(0)	52(0)	422(4)	410(6)
	60(0)	59(0)	431(5)	418(3)
	64(0)	60(0)	440(4)	421(2)
	67(0)	63(0)	445(1)	429(1)
	69(0)	65(0)	453(0)	441(2)
	71(0)	66(0)	460(0)	444(1)
	78(1)	74(0)	481(43)	466(35)
	79(0)	75(0)	499(1)	474(1)
	81(0)	79(0)	521(16)	491(9)
	96(0)	90(0)	535(45)	509(26)
	118(0)	103(0)	539(36)	512(17)
	131(0)	117(0)	548(30)	517(30)
	170(0)	162(0)	559(47)	529(30)
	198(0)	175(0)	600(63)	570(46)
	322(0)	295(6)	1864(429)	1769(333)
	331(8)	307(0)	1944(278)	1847(353)
	333(15)	325(0)	2058(106)	1939(21)
	339(2)	330(0)	2063(671)	1949(724)
	344(12)	332(0)	2083(1254)	1956(552)
	345(0)	335(7)	2092(1371)	1968(2919)
	350(0)	335(6)	2095(3478)	1969(849)
	355(7)	344(4)	2117(59)	1980(70)
	358(7)	350(2)	2134(3821)	2003(3467)
	365(43)	359(16)	2188(6)	2053(8)

Table S19. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structre **10T-3** of triplet $Nb_2(CO)_{10}$ with C_i symmetry.

	MPW1PW91	BP86		MPW1PW91	BP86
AG	34(0)	26(0)	AU	5i	10i
	47(0)	45(0)		21(0)	22(0)
	54(0)	52(0)		40(0)	35(0)
	64(0)	57(0)		52(0)	53(0)
	66(0)	62(0)		59(0)	57(0)
	69(0)	65(0)		66(1)	63(0)
	79(0)	75(0)		72(1)	70(0)
	90(0)	85(0)		77(2)	76(1)
	113(0)	103(0)		82(0)	77(0)
	156(0)	155(0)		121(2)	108(1)
	330(0)	316(0)		309(1)	295(0)
	332(0)	325(0)		332(3)	316(0)
	337(0)	329(0)		341(30)	334(1)
	353(0)	346(0)		351(0)	342(20)
	361(0)	360(0)		358(33)	358(26)
	368(0)	364(0)		367(58)	361(31)
	397(0)	386(0)		388(21)	373(17)
	416(0)	406(0)		405(68)	407(22)
	443(0)	419(0)		434(8)	420(6)
	447(0)	433(0)		450(5)	431(0)
	453(0)	440(0)		456(7)	443(6)
	482(0)	462(0)		499(25)	477(6)
	523(0)	497(0)		505(44)	482(51)
	531(0)	506(0)		529(61)	507(43)
	551(0)	529(0)		562(65)	540(58)
	1966(0)	1850(0)		1981(1335)	1862(876)
	2060(0)	1939(0)		2069(2621)	1948(1615)
	2073(0)	1950(0)		2089(1377)	1968(981)
	2103(0)	1975(0)		2099(2918)	1970(2598)
	2187(0)	2053(0)		2127(3972)	2001(3396)

Table S20. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **10T-4** of triplet $Nb_2(CO)_{10}$ with C_{2v} symmetry.

	MPW1PW91	BP86
A1	49(0)	47(0)
	60(0)	55(0)
	67(0)	63(0)
	81(1)	78(0)
	97(0)	94(0)
	201(12)	208(2)
	346(57)	343(16)
	349(0)	351(12)
	381(2)	369(9)
	403(12)	386(9)
	425(5)	418(2)
	438(11)	421(20)
	487(0)	465(5)
	526(23)	498(4)
	552(11)	538(0)
	584(74)	547(61)
	1850(532)	1735(70)
	2082(2818)	1951(886)
	2094(3)	1970(240)
	2146(1909)	1998(3644)
	2187(0)	2049(56)
B1	29(0)	27(0)
	55(0)	55(0)
	69(0)	65(0)
	78(0)	75(0)
	99(0)	109(0)
	318(40)	317(0)
	335(0)	327(21)
	356(1)	346(8)
	389(39)	375(26)
	447(5)	421(2)
	518(22)	501(16)
	593(51)	559(35)
	2056(935)	1943(66)
	2112(2729)	1969(3016)

	MPW1PW91	BP86
A2	21(0)	20(0)
	51(0)	51(0)
	67(0)	64(0)
	89(0)	88(0)
	313(0)	306(0)
	329(0)	311(0)
	437(0)	410(0)
	459(0)	444(0)
	506(0)	473(0)
B2	31(0)	27(0)
	42(0)	39(0)
	66(1)	61(0)
	83(0)	80(0)
	153(2)	185(0)
	325(1)	311(0)
	349(17)	344(10)
	370(20)	374(0)
	391(5)	380(12)
	417(19)	413(0)
	437(15)	424(25)
	491(0)	459(0)
	572(83)	532(54)
	1818(975)	1720(695)
	2034(1001)	1922(667)
	2115(952)	1982(877)

Table S21 Cartesian coordinates of **12S-1,12S-2,12S-3,12S-4**

12S-1 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	-1.654661
41	0.000000	0.000000	1.706590
6	0.529159	-1.095123	-3.350111
8	0.830510	-1.692779	-4.288864
6	1.988830	0.769997	1.617720
8	3.063345	1.184899	1.591786
6	2.119535	-0.321270	-1.434600
8	3.254514	-0.470321	-1.351049
6	0.000000	1.272901	3.385546
8	0.065073	1.948961	4.316252
6	0.816166	1.961303	-1.272462
8	1.298179	2.992380	-1.118429
6	-1.038246	1.736114	0.987946
8	-1.678714	2.669848	0.766708
6	-2.119535	0.321270	-1.434600
8	-3.254514	0.470321	-1.351049
6	-1.988830	-0.769997	1.617720
8	-3.063345	-1.184899	1.591786
6	1.038246	-1.736114	0.987946
8	1.678714	-2.669848	0.766708
6	-0.816166	-1.961303	-1.272462
8	-1.298179	-2.992380	-1.118429
6	-0.529159	1.095123	-3.350111
8	-0.830510	1.692779	-4.288864
6	0.000000	-1.272901	3.385546
8	-0.065073	-1.948961	4.316252

12S-1 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	-1.689819
41	0.000000	0.000000	1.739034
6	2.114048	-0.383757	-1.487440
8	3.263470	-0.567355	-1.414028
6	0.466841	-1.130097	-3.385548
8	0.744799	-1.748522	-4.340761
6	-0.466841	1.130097	-3.385548
8	-0.744799	1.748522	-4.340761
6	0.865819	1.939974	-1.273156
8	1.390820	2.970886	-1.119896
6	-0.990021	1.758963	0.984990
8	-1.624066	2.721628	0.772004
6	2.012427	0.728805	1.672122
8	3.113934	1.124722	1.663808
6	0.990021	-1.758963	0.984990
8	1.624066	-2.721628	0.772004
6	0.000000	-1.281250	3.418389
8	-0.072439	-1.964934	4.365742
6	-0.865819	-1.939974	-1.273156
8	-1.390820	-2.970886	-1.119896
6	-2.114048	0.383757	-1.487440
8	-3.263470	0.567355	-1.414028
6	-2.012427	-0.728805	1.672122
8	-3.113934	-1.124722	1.663808
6	0.000000	1.281250	3.418389
8	0.072439	1.964934	4.365742

12S-2 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.676531
41	0.000000	0.000000	-1.676531
6	-0.564026	2.062830	1.520383
8	-0.856150	3.173502	1.462550
6	-1.206019	0.279383	3.365333
8	-1.851737	0.469625	4.301200
6	1.206019	-0.279383	3.365333
8	1.851737	-0.469625	4.301200
6	1.847181	0.960582	1.126965
8	2.822538	1.539038	0.930781
6	1.847181	-0.960582	-1.126965
8	2.822538	-1.539038	-0.930781
6	0.564026	2.062830	-1.520383
8	0.856150	3.173502	-1.462550
6	-1.847181	0.960582	-1.126965
8	-2.822538	1.539038	-0.930781
6	-1.206019	-0.279383	-3.365333
8	-1.851737	-0.469625	-4.301200
6	-1.847181	-0.960582	1.126965
8	-2.822538	-1.539038	0.930781
6	0.564026	-2.062830	1.520383
8	0.856150	-3.173502	1.462550
6	-0.564026	-2.062830	-1.520383
8	-0.856150	-3.173502	-1.462550
6	1.206019	0.279383	-3.365333
8	1.851737	0.469625	-4.301200

12S-2 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.715526
41	0.000000	0.000000	-1.715526
6	-0.583390	2.064313	1.596221
8	-0.888862	3.191567	1.560125
6	-1.234290	0.208075	3.401995
8	-1.895773	0.375254	4.353806
6	1.234290	-0.208075	3.401995
8	1.895773	-0.375254	4.353806
6	1.836949	0.957879	1.101620
8	2.820699	1.559919	0.908989
6	1.836949	-0.957879	-1.101620
8	2.820699	-1.559919	-0.908989
6	0.583390	2.064313	-1.596221
8	0.888862	3.191567	-1.560125
6	-1.836949	0.957879	-1.101620
8	-2.820699	1.559919	-0.908989
6	-1.234290	-0.208075	-3.401995
8	-1.895773	-0.375254	-4.353806
6	-1.836949	-0.957879	1.101620
8	-2.820699	-1.559919	0.908989
6	0.583390	-2.064313	1.596221
8	0.888862	-3.191567	1.560125
6	-0.583390	-2.064313	-1.596221
8	-0.888862	-3.191567	-1.560125
6	1.234290	0.208075	-3.401995
8	1.895773	0.375254	-4.353806

12S-3 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.805524
41	0.000000	0.000000	-1.805524
6	0.000000	-1.740670	3.063559
8	0.000000	-2.655619	3.758860
6	0.000000	2.007061	1.064369
8	0.000000	3.131661	0.811396
6	1.507464	0.870335	3.063559
8	2.299833	1.327809	3.758860
6	1.738166	-1.003531	1.064369
8	2.712098	-1.565831	0.811396
6	1.738166	1.003531	-1.064369
8	2.712098	1.565831	-0.811396
6	1.507464	-0.870335	-3.063559
8	2.299833	-1.327809	-3.758860
6	0.000000	-2.007061	-1.064369
8	0.000000	-3.131661	-0.811396
6	-1.507464	-0.870335	-3.063559
8	-2.299833	-1.327809	-3.758860
6	-1.738166	-1.003531	1.064369
8	-2.712098	-1.565831	0.811396
6	-1.507464	0.870335	3.063559
8	-2.299833	1.327809	3.758860
6	0.000000	1.740670	-3.063559
8	0.000000	2.655619	-3.758860
6	-1.738166	1.003531	-1.064369
8	-2.712098	1.565831	-0.811396

12S-3 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.833920
41	0.000000	0.000000	-1.833920
6	0.000000	-1.731730	3.106800
8	0.000000	-2.649336	3.829136
6	0.000000	2.018423	1.096252
8	0.000000	3.164892	0.859336
6	1.499722	0.865865	3.106800
8	2.294392	1.324668	3.829136
6	1.748005	-1.009211	1.096252
8	2.740877	-1.582446	0.859336
6	1.748005	1.009211	-1.096252
8	2.740877	1.582446	-0.859336
6	1.499722	-0.865865	-3.106800
8	2.294392	-1.324668	-3.829136
6	0.000000	-2.018423	-1.096252
8	0.000000	-3.164892	-0.859336
6	-1.499722	-0.865865	-3.106800
8	-2.294392	-1.324668	-3.829136
6	-1.748005	-1.009211	1.096252
8	-2.740877	-1.582446	0.859336
6	-1.499722	0.865865	3.106800
8	-2.294392	1.324668	3.829136
6	0.000000	1.731730	-3.106800
8	0.000000	2.649336	-3.829136
6	-1.748005	1.009211	-1.096252
8	-2.740877	1.582446	-0.859336

12S-4 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	1.701240	0.014369
41	0.000000	-1.701240	0.014369
6	0.000000	1.531882	2.150763
8	0.000000	1.557649	3.300870
6	0.000000	2.041072	-2.086848
8	0.000000	2.272134	-3.213907
6	2.033552	2.202159	0.441984
8	3.089539	2.540768	0.741740
6	1.414230	0.000000	-0.831784
8	2.377364	0.000000	-1.494039
6	2.033552	-2.202159	0.441984
8	3.089539	-2.540768	0.741740
6	0.000000	-3.786062	-0.077862
8	0.000000	-4.934750	-0.178720
6	0.000000	-1.531882	2.150763
8	0.000000	-1.557649	3.300870
6	-2.033552	-2.202159	0.441984
8	-3.089539	-2.540768	0.741740
6	-2.033552	2.202159	0.441984
8	-3.089539	2.540768	0.741740
6	0.000000	3.786062	-0.077862
8	0.000000	4.934750	-0.178720
6	0.000000	-2.041072	-2.086848
8	0.000000	-2.272134	-3.213907
6	-1.414230	0.000000	-0.831784
8	-2.377364	0.000000	-1.494039

12S-4 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	1.719549	-0.006905
41	0.000000	-1.719549	-0.006905
6	0.000000	1.550057	-2.148225
8	0.000000	1.582939	-3.316741
6	0.000000	2.067564	2.104192
8	0.000000	2.310609	3.247234
6	2.028239	2.231619	-0.458504
8	3.091903	2.584398	-0.786610
6	1.424653	0.000000	0.832685
8	2.404294	0.000000	1.501697
6	2.028239	-2.231619	-0.458504
8	3.091903	-2.584398	-0.786610
6	0.000000	-3.806168	0.096943
8	0.000000	-4.973292	0.199978
6	0.000000	-1.550057	-2.148225
8	0.000000	-1.582939	-3.316741
6	-2.028239	-2.231619	-0.458504
8	-3.091903	-2.584398	-0.786610
6	-2.028239	2.231619	-0.458504
8	-3.091903	2.584398	-0.786610
6	0.000000	3.806168	0.096943
8	0.000000	4.973292	0.199978
6	0.000000	-2.067564	2.104192
8	0.000000	-2.310609	3.247234
6	-1.424653	0.000000	0.832685
8	-2.404294	0.000000	1.501697

Table S22 Cartesian coordinates of **11S-1,11S-2,11S-3,11S-4**

11S-1 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.109744	-0.975790	0.939786
8	3.887410	-1.538584	1.582166
6	1.396174	0.536619	1.739888
8	1.300846	0.882468	2.836579
6	1.997824	2.093564	-0.191984
8	2.185557	3.226420	-0.153370
6	-3.798717	-0.202837	0.734588
8	-4.889973	-0.342512	1.057457
6	-2.835591	1.287135	-1.384777
8	-3.401754	1.992193	-2.096336
6	-1.410311	1.855045	1.032784
8	-1.238814	2.853067	1.582276
6	-2.158462	-1.792785	-1.043268
8	-2.368015	-2.779455	-1.602918
6	3.560657	0.238546	-1.198320
8	4.582657	0.416111	-1.695648
6	1.211216	-2.127009	-0.511769
8	0.994087	-3.245496	-0.633211
6	-0.329000	0.222988	-1.456807
8	0.513631	0.305328	-2.305391
6	-1.126908	-1.160144	1.666189
8	-0.899097	-1.809148	2.587955
41	-1.768518	0.031560	-0.029785
41	1.694566	-0.020222	-0.244223

11-1 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.151249	-0.928726	0.978563
8	3.937952	-1.474356	1.656943
6	1.386470	0.572392	1.720413
8	1.287119	0.945321	2.827556
6	2.037033	2.096851	-0.241292
8	2.228188	3.248921	-0.222726
6	-3.874254	-0.229366	0.568681
8	-5.009181	-0.389548	0.784516
6	-2.766358	1.354732	-1.375257
8	-3.290086	2.118473	-2.089181
6	-1.512147	1.823912	1.125728
8	-1.400332	2.817549	1.732708
6	-2.176585	-1.800415	-1.054522
8	-2.391825	-2.799776	-1.626172
6	3.606158	0.220439	-1.209716
8	4.649294	0.397829	-1.707502
6	1.293391	-2.142069	-0.466497
8	1.105832	-3.288062	-0.563791
6	-0.319734	0.183146	-1.430852
8	0.505102	0.253415	-2.322676
6	-1.210606	-1.172977	1.705846
8	-1.000838	-1.812423	2.660423
41	-1.800744	0.022398	-0.014015
41	1.735927	-0.022551	-0.253482

11S-2 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.159563	1.588918	0.000000
41	0.048153	-1.482137	0.000000
6	1.552701	-0.731790	1.334623
8	2.428615	-0.411092	2.013459
6	0.078172	1.621208	-2.118870
8	-0.039553	1.687875	-3.266525
6	1.577252	3.233869	0.000000
8	2.226043	4.180961	0.000000
6	0.609086	-3.094837	-1.230142
8	0.935022	-3.962596	-1.912740
6	-1.625974	-1.709043	1.381352
8	-2.507319	-1.826324	2.101887
6	-1.625974	-1.709043	-1.381352
8	-2.507319	-1.826324	-2.101887
6	0.609086	-3.094837	1.230142
8	0.935022	-3.962596	1.912740
6	0.078172	1.621208	2.118870
8	-0.039553	1.687875	3.266525
6	-1.158480	3.177976	0.000000
8	-1.887326	4.074019	0.000000
6	1.552701	-0.731790	-1.334623
8	2.428615	-0.411092	-2.013459
6	-1.780308	0.822113	0.000000
8	-2.936618	0.668266	0.000000

11S-2 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.143500	1.588794	0.000000
41	0.041377	-1.488111	0.000000
6	1.467739	-0.612353	1.370654
8	2.344231	-0.302979	2.088379
6	0.031009	1.706087	-2.125135
8	-0.111547	1.850688	-3.280784
6	1.585816	3.197188	0.000000
8	2.277141	4.138309	0.000000
6	0.745439	-3.042499	-1.230740
8	1.163995	-3.885833	-1.925424
6	-1.607732	-1.882591	1.375873
8	-2.496139	-2.092793	2.096788
6	-1.607732	-1.882591	-1.375873
8	-2.496139	-2.092793	-2.096788
6	0.745439	-3.042499	1.230740
8	1.163995	-3.885833	1.925424
6	0.031009	1.706087	2.125135
8	-0.111547	1.850688	3.280784
6	-1.201738	3.160769	0.000000
8	-1.964322	4.051839	0.000000
6	1.467739	-0.612353	-1.370654
8	2.344231	-0.302979	-2.088379
6	-1.789376	0.740369	0.000000
8	-2.962103	0.578974	0.000000

11S-3 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	1.536843	0.050767
41	0.000000	-1.536843	0.050767
6	0.000000	0.000000	1.857394
8	0.000000	0.000000	3.011128
6	2.008771	1.724187	0.718515
8	3.089957	1.852039	1.096798
6	-0.237957	3.125877	1.479193
8	-0.292757	4.034070	2.180664
6	2.122441	-1.484908	-0.381968
8	3.249386	-1.554284	-0.594015
6	0.237957	-3.125877	1.479193
8	0.292757	-4.034070	2.180664
6	1.090034	0.945708	-1.640982
8	1.743794	0.809891	-2.585288
6	-2.008771	-1.724187	0.718515
8	-3.089957	-1.852039	1.096798
6	-2.122441	1.484908	-0.381968
8	-3.249386	1.554284	-0.594015
6	-0.089993	3.233452	-1.156731
8	-0.156508	4.172826	-1.823946
6	-1.090034	-0.945708	-1.640982
8	-1.743794	-0.809891	-2.585288
6	0.089993	-3.233452	-1.156731
8	0.156508	-4.172826	-1.823946

11S-3 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	1.558322	0.040732
41	0.000000	-1.558322	0.040732
6	0.000000	0.000000	1.822818
8	0.000000	0.000000	2.998720
6	2.008371	1.754481	0.733122
8	3.096960	1.899232	1.138571
6	-0.212896	3.149006	1.464513
8	-0.249935	4.075630	2.174521
6	2.134296	-1.544808	-0.357214
8	3.282617	-1.650126	-0.539777
6	0.212896	-3.149006	1.464513
8	0.249935	-4.075630	2.174521
6	1.118336	0.943867	-1.641090
8	1.797991	0.809858	-2.589097
6	-2.008371	-1.754481	0.733122
8	-3.096960	-1.899232	1.138571
6	-2.134296	1.544808	-0.357214
8	-3.282617	1.650126	-0.539777
6	-0.068547	3.262312	-1.169197
8	-0.122192	4.216433	-1.848489
6	-1.118336	-0.943867	-1.641090
8	-1.797991	-0.809858	-2.589097
6	0.068547	-3.262312	-1.169197
8	0.122192	-4.216433	-1.848489

11S-4 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	-0.394090	1.952052	0.000000
41	0.117519	-1.413846	0.000000
6	1.560498	1.308883	0.000000
8	2.720903	1.195764	0.000000
6	1.370273	-0.955130	1.711105
8	2.009358	-0.750220	2.639337
6	0.509336	3.898213	0.000000
8	0.962602	4.955074	0.000000
6	-1.198791	-1.369328	1.713963
8	-1.868667	-1.372279	2.644981
6	-0.350315	1.934880	2.111503
8	-0.287914	1.911417	3.266871
6	-1.198791	-1.369328	-1.713963
8	-1.868667	-1.372279	-2.644981
6	-2.130133	0.720553	0.000000
8	-3.227659	0.348216	0.000000
6	1.370273	-0.955130	-1.711105
8	2.009358	-0.750220	-2.639337
6	1.557500	-2.918747	0.000000
8	2.355504	-3.751044	0.000000
6	-0.350315	1.934880	-2.111503
8	-0.287914	1.911417	-3.266871
6	-0.818804	-3.272752	0.000000
8	-1.340022	-4.301896	0.000000

11S-4 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	-0.362466	1.976856	0.000000
41	0.093868	-1.464142	0.000000
6	1.610290	1.369055	0.000000
8	2.788007	1.260602	0.000000
6	1.317025	-0.917182	1.708455
8	1.954190	-0.684226	2.654909
6	0.378239	3.987349	0.000000
8	0.731360	5.102217	0.000000
6	-1.229146	-1.498770	1.714986
8	-1.910810	-1.542781	2.659039
6	-0.340908	2.001471	2.120970
8	-0.306676	2.029898	3.295734
6	-1.229146	-1.498770	-1.714986
8	-1.910810	-1.542781	-2.659039
6	-2.039205	0.668186	0.000000
8	-3.170823	0.329826	0.000000
6	1.317025	-0.917182	-1.708455
8	1.954190	-0.684226	-2.654909
6	1.628202	-2.876892	0.000000
8	2.489370	-3.670825	0.000000
6	-0.340908	2.001471	-2.120970
8	-0.306676	2.029898	-3.295734
6	-0.730496	-3.380731	0.000000
8	-1.190485	-4.458762	0.000000

Table S23 Cartesian coordinates of **11T-1, 11T-2, 11T-3**

11T-1 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.029391	-1.561017	0.000000
41	0.047840	1.567520	0.000000
6	1.785978	-0.316488	0.000000
8	2.935192	-0.117185	0.000000
6	1.233225	-2.504296	1.499283
8	1.881500	-3.039055	2.284344
6	1.936530	2.612399	0.000000
8	2.882279	3.263772	0.000000
6	-0.828569	3.496453	0.000000
8	-1.308917	4.542123	0.000000
6	-1.153276	-3.350416	0.000000
8	-1.757645	-4.326611	0.000000
6	-1.263337	-1.045367	1.633332
8	-1.962170	-0.910817	2.540291
6	1.233225	-2.504296	-1.499283
8	1.881500	-3.039055	-2.284344
6	0.110793	1.661241	2.150509
8	0.163878	1.765408	3.293873
6	-2.051270	1.174105	0.000000
8	-3.201202	1.094097	0.000000
6	0.110793	1.661241	-2.150509
8	0.163878	1.765408	-3.293873
6	-1.263337	-1.045367	-1.633332
8	-1.962170	-0.910817	-2.540291

11T-1 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.025139	-1.576713	0.000000
41	0.052172	1.573861	0.000000
6	1.768969	-0.233684	0.000000
8	2.943473	-0.075287	0.000000
6	1.273116	-2.505628	1.481409
8	1.950883	-3.055023	2.258081
6	1.887311	2.705515	0.000000
8	2.812537	3.417661	0.000000
6	-0.847374	3.490633	0.000000
8	-1.343808	4.549823	0.000000
6	-1.103007	-3.392069	0.000000
8	-1.691973	-4.400010	0.000000
6	-1.294229	-1.098286	1.637855
8	-2.011423	-0.992871	2.556010
6	1.273116	-2.505628	-1.481409
8	1.950883	-3.055023	-2.258081
6	0.115050	1.676212	2.150399
8	0.170138	1.797698	3.311550
6	-2.049078	1.169678	0.000000
8	-3.219164	1.109320	0.000000
6	0.115050	1.676212	-2.150399
8	0.170138	1.797698	-3.311550
6	-1.294229	-1.098286	-1.637855
8	-2.011423	-0.992871	-2.556010

11T-2 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	1.770969
8	0.000000	0.000000	2.938984
6	-0.682027	-2.663045	1.727970
8	-1.016496	-3.320414	2.608752
6	0.682027	2.663045	1.727970
8	1.016496	3.320414	2.608752
6	-2.001413	1.900285	0.736528
8	-3.060817	2.130730	1.118849
6	2.001413	-1.900285	0.736528
8	3.060817	-2.130730	1.118849
6	-2.050990	-1.373350	-0.594099
8	-3.155708	-1.359983	-0.914800
6	0.918201	-1.046136	-1.826990
8	1.449821	-0.939358	-2.845495
6	-0.918201	1.046136	-1.826990
8	-1.449821	0.939358	-2.845495
6	0.066037	3.378818	-1.008350
8	0.115093	4.382081	-1.567614
6	2.050990	1.373350	-0.594099
8	3.155708	1.359983	-0.914800
6	-0.066037	-3.378818	-1.008350
8	-0.115093	-4.382081	-1.567614
41	0.000000	1.529431	0.037153
41	0.000000	-1.529431	0.037153

11T-2 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	1.767566
8	0.000000	0.000000	2.953435
6	-0.698652	-2.707443	1.710673
8	-1.041568	-3.399744	2.586160
6	0.698652	2.707443	1.710673
8	1.041568	3.399744	2.586160
6	-1.982437	1.980587	0.769796
8	-3.040017	2.260118	1.179914
6	1.982437	-1.980587	0.769796
8	3.040017	-2.260118	1.179914
6	-2.047403	-1.393011	-0.617449
8	-3.167268	-1.398986	-0.952665
6	0.938238	-1.078444	-1.831752
8	1.477369	-0.990325	-2.867848
6	-0.938238	1.078444	-1.831752
8	-1.477369	0.990325	-2.867848
6	0.075616	3.409784	-0.994146
8	0.130589	4.435175	-1.552434
6	2.047403	1.393011	-0.617449
8	3.167268	1.398986	-0.952665
6	-0.075616	-3.409784	-0.994146
8	-0.130589	-4.435175	-1.552434
41	0.000000	1.555740	0.036971
41	0.000000	-1.555740	0.036971

11T-3 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	1.870049	0.597811
8	0.000000	3.003683	0.352109
6	0.000000	1.449957	3.203504
8	0.000000	2.207436	4.066672
6	1.605049	1.417709	-1.740197
8	2.479034	2.143616	-1.917658
6	-1.605049	1.417709	-1.740197
8	-2.479034	2.143616	-1.917658
6	2.155501	0.000000	1.600313
8	3.305440	0.000000	1.589006
6	-2.155501	0.000000	1.600313
8	-3.305440	0.000000	1.589006
6	0.000000	-1.870049	0.597811
8	0.000000	-3.003683	0.352109
6	-1.605049	-1.417709	-1.740197
8	-2.479034	-2.143616	-1.917658
6	0.000000	0.000000	-3.674421
8	0.000000	0.000000	-4.825022
6	1.605049	-1.417709	-1.740197
8	2.479034	-2.143616	-1.917658
6	0.000000	-1.449957	3.203504
8	0.000000	-2.207436	4.066672
41	0.000000	0.000000	1.622144
41	0.000000	0.000000	-1.553062

11T-3 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	1.869016	0.596317
8	0.000000	3.022103	0.351820
6	0.000000	1.446240	3.232280
8	0.000000	2.210771	4.114229
6	1.599864	1.423475	-1.784629
8	2.478777	2.162031	-2.001774
6	-1.599864	1.423475	-1.784629
8	-2.478777	2.162031	-2.001774
6	2.159207	0.000000	1.657437
8	3.327517	0.000000	1.681143
6	-2.159207	0.000000	1.657437
8	-3.327517	0.000000	1.681143
6	0.000000	-1.869016	0.596317
8	0.000000	-3.022103	0.351820
6	-1.599864	-1.423475	-1.784629
8	-2.478777	-2.162031	-2.001774
6	0.000000	0.000000	-3.681185
8	0.000000	0.000000	-4.850451
6	1.599864	-1.423475	-1.784629
8	2.478777	-2.162031	-2.001774
6	0.000000	-1.446240	3.232280
8	0.000000	-2.210771	4.114229
41	0.000000	0.000000	1.647197
41	0.000000	0.000000	-1.559609

Table S24 Cartesian coordinates of **10S-1,10S-2,10S-3,10S-4,10S-5**

10S-1 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.908380	0.558526	0.000000
8	3.047720	0.336049	0.000000
6	-0.964281	0.578161	1.686631
8	-1.512854	0.353730	2.684171
6	0.851490	2.773004	1.481641
8	1.316066	3.469051	2.266685
6	1.242763	-2.407078	-1.228963
8	1.961035	-2.987492	-1.920829
6	1.242763	-2.407078	1.228963
8	1.961035	-2.987492	1.920829
6	-1.200192	-2.529725	-1.217121
8	-1.857655	-3.184048	-1.903061
6	-0.964281	0.578161	-1.686631
8	-1.512854	0.353730	-2.684171
6	0.851490	2.773004	-1.481641
8	1.316066	3.469051	-2.266685
6	-1.200192	-2.529725	1.217121
8	-1.857655	-3.184048	1.903061
6	-1.737523	2.774092	0.000000
8	-2.651785	3.467267	0.000000
41	-0.026635	-1.324311	0.000000
41	-0.018620	1.475179	0.000000

10S-1 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.908820	0.545746	0.000000
8	3.066016	0.319350	0.000000
6	-0.962131	0.564331	1.688456
8	-1.515747	0.332238	2.703039
6	0.845368	2.803226	1.474025
8	1.313810	3.519988	2.265530
6	1.242442	-2.420278	-1.230105
8	1.970696	-3.011454	-1.934268
6	1.242442	-2.420278	1.230105
8	1.970696	-3.011454	1.934268
6	-1.197698	-2.547837	-1.214067
8	-1.864585	-3.217753	-1.908150
6	-0.962131	0.564331	-1.688456
8	-1.515747	0.332238	-2.703039
6	0.845368	2.803226	-1.474025
8	1.313810	3.519988	-2.265530
6	-1.197698	-2.547837	1.214067
8	-1.864585	-3.217753	1.908150
6	-1.733722	2.798223	0.000000
8	-2.658871	3.507969	0.000000
41	-0.026422	-1.332056	0.000000
41	-0.020171	1.491959	0.000000

10S-2 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.144209	0.000000	1.565616
8	-3.294974	0.000000	1.599487
6	0.000000	1.840740	0.440085
8	0.000000	2.977940	0.199384
6	0.000000	1.454625	3.095756
8	0.000000	2.221656	3.949318
6	-1.219751	-1.220446	-2.499513
8	-1.914087	-1.900905	-3.121059
6	-1.219751	1.220446	-2.499513
8	-1.914087	1.900905	-3.121059
6	1.219751	-1.220446	-2.499513
8	1.914087	-1.900905	-3.121059
6	0.000000	-1.840740	0.440085
8	0.000000	-2.977940	0.199384
6	0.000000	-1.454625	3.095756
8	0.000000	-2.221656	3.949318
6	1.219751	1.220446	-2.499513
8	1.914087	1.900905	-3.121059
6	2.144209	0.000000	1.565616
8	3.294974	0.000000	1.599487
41	0.000000	0.000000	-1.351902
41	0.000000	0.000000	1.514675

10S-2 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.151246	0.000000	1.586418
8	-3.319712	0.000000	1.629362
6	0.000000	1.837950	0.425842
8	0.000000	2.993534	0.178414
6	0.000000	1.452716	3.114793
8	0.000000	2.229631	3.984482
6	-1.220531	-1.218250	-2.515847
8	-1.928911	-1.906605	-3.148601
6	-1.220531	1.218250	-2.515847
8	-1.928911	1.906605	-3.148601
6	1.220531	-1.218250	-2.515847
8	1.928911	-1.906605	-3.148601
6	0.000000	-1.837950	0.425842
8	0.000000	-2.993534	0.178414
6	0.000000	-1.452716	3.114793
8	0.000000	-2.229631	3.984482
6	1.220531	1.218250	-2.515847
8	1.928911	1.906605	-3.148601
6	2.151246	0.000000	1.586418
8	3.319712	0.000000	1.629362
41	0.000000	0.000000	-1.361723
41	0.000000	0.000000	1.530865

10S-3 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.543118	-2.826670	-0.039607
8	2.423160	-3.570115	-0.086300
6	1.818322	-0.309192	-0.526912
8	2.912748	-0.061823	-0.836522
6	1.622275	2.649210	0.478694
8	2.516792	3.323459	0.729070
6	0.475720	-1.412568	2.092346
8	0.742494	-1.526564	3.205143
6	-0.475720	1.412568	2.092346
8	-0.742494	1.526564	3.205143
6	-1.622275	-2.649210	0.478694
8	-2.516792	-3.323459	0.729070
6	-1.818322	0.309192	-0.526912
8	-2.912748	0.061823	-0.836522
6	-0.310783	-2.131932	-1.985288
8	-0.475720	-2.613493	-3.014047
6	0.310783	2.131932	-1.985288
8	0.475720	2.613493	-3.014047
6	-1.543118	2.826670	-0.039607
8	-2.423160	3.570115	-0.086300
41	-0.040799	1.362569	-0.002297
41	0.040799	-1.362569	-0.002297

10S-3 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.566115	-2.825493	-0.040138
8	2.469111	-3.570231	-0.083596
6	1.804915	-0.291362	-0.566397
8	2.910281	-0.036873	-0.899682
6	1.581606	2.707398	0.496909
8	2.469111	3.416441	0.765964
6	0.480574	-1.420358	2.087745
8	0.753668	-1.550501	3.216519
6	-0.480574	1.420358	2.087745
8	-0.753668	1.550501	3.216519
6	-1.581606	-2.707398	0.496909
8	-2.469111	-3.416441	0.765964
6	-1.804915	0.291362	-0.566397
8	-2.910281	0.036873	-0.899682
6	-0.315925	-2.235058	-1.956329
8	-0.485908	-2.785520	-2.971170
6	0.315925	2.235058	-1.956329
8	0.485908	2.785520	-2.971170
6	-1.566115	2.825493	-0.040138
8	-2.469111	3.570231	-0.083596
41	-0.038171	1.385468	-0.008659
41	0.038171	-1.385468	-0.008659

10S-4 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.112580	-1.731940	2.121967
8	-0.112580	-1.984378	3.242201
6	1.839924	-0.477860	0.000000
8	2.993432	-0.319910	0.000000
6	1.881173	2.573471	0.000000
8	2.828971	3.220026	0.000000
6	0.112580	1.731940	2.121967
8	0.112580	1.984378	3.242201
6	-1.277071	2.959325	0.000000
8	-2.090164	3.777817	0.000000
6	1.277071	-2.959325	0.000000
8	2.090164	-3.777817	0.000000
6	-0.112580	-1.731940	-2.121967
8	-0.112580	-1.984378	-3.242201
6	-1.881173	-2.573471	0.000000
8	-2.828971	-3.220026	0.000000
6	-1.839924	0.477860	0.000000
8	-2.993432	0.319910	0.000000
6	0.112580	1.731940	-2.121967
8	0.112580	1.984378	-3.242201
41	0.085758	1.368118	0.000000
41	-0.085758	-1.368118	0.000000

10S-4 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.050457	-1.801172	2.114875
8	-0.050457	-2.102073	3.242503
6	1.854103	-0.381554	0.000000
8	3.016618	-0.163585	0.000000
6	1.737394	2.711847	0.000000
8	2.653259	3.434920	0.000000
6	0.050457	1.801172	2.114875
8	0.050457	2.102073	3.242503
6	-1.421363	2.907361	0.000000
8	-2.288828	3.695457	0.000000
6	1.421363	-2.907361	0.000000
8	2.288828	-3.695457	0.000000
6	-0.050457	-1.801172	-2.114875
8	-0.050457	-2.102073	-3.242503
6	-1.737394	-2.711847	0.000000
8	-2.653259	-3.434920	0.000000
6	-1.854103	0.381554	0.000000
8	-3.016618	0.163585	0.000000
6	0.050457	1.801172	-2.114875
8	0.050457	2.102073	-3.242503
41	0.031221	1.394129	0.000000
41	-0.031221	-1.394129	0.000000

10S-5 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.745654
41	0.000000	0.000000	-1.651042
6	2.106356	-0.326064	-1.653306
8	3.245042	-0.482147	-1.723124
6	-2.106356	0.326064	-1.653306
8	-3.245042	0.482147	-1.723124
6	0.632647	1.129374	-3.288261
8	1.043460	1.724783	-4.186761
6	-0.632647	-1.129374	-3.288261
8	-1.043460	-1.724783	-4.186761
6	2.106594	0.329639	1.739507
8	3.243929	0.511883	1.727702
6	-0.080220	1.510905	0.332496
8	0.000000	2.220966	-0.614150
6	-2.106594	-0.329639	1.739507
8	-3.243929	-0.511883	1.727702
6	-0.462914	1.410181	3.357146
8	-0.775170	2.134794	4.188204
6	0.462914	-1.410181	3.357146
8	0.775170	-2.134794	4.188204
6	0.080220	-1.510905	0.332496
8	0.000000	-2.220966	-0.614150

10S-5 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.768725
41	0.000000	0.000000	-1.669140
6	2.114711	-0.309744	-1.686404
8	3.272843	-0.456900	-1.772673
6	-2.114711	0.309744	-1.686404
8	-3.272843	0.456900	-1.772673
6	0.644160	1.116515	-3.308503
8	1.066524	1.714193	-4.225024
6	-0.644160	-1.116515	-3.308503
8	-1.066524	-1.714193	-4.225024
6	2.099614	0.423306	1.779030
8	3.245177	0.659584	1.788245
6	-0.106504	1.507053	0.328319
8	0.000000	2.229860	-0.630861
6	-2.099614	-0.423306	1.779030
8	-3.245177	-0.659584	1.788245
6	-0.569815	1.367131	3.374170
8	-0.957685	2.068309	4.220167
6	0.569815	-1.367131	3.374170
8	0.957685	-2.068309	4.220167
6	0.106504	-1.507053	0.328319
8	0.000000	-2.229860	-0.630861

Table S25 Cartesian coordinates of **10T-1,10T-2,10T-3,10T-4**

10T-1 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.402341	2.094227	0.545986
8	1.356619	3.199537	0.865369
6	0.204900	0.306546	-1.618711
8	-0.652094	0.424675	-2.425361
6	3.026579	0.689977	-1.506991
8	3.805032	1.037301	-2.276327
6	-2.490745	-0.301791	1.771072
8	-2.994847	-0.466709	2.795270
6	-1.869877	2.094780	0.248362
8	-2.115178	3.199546	0.459137
6	-1.659164	-2.127008	-0.332862
8	-1.767331	-3.269981	-0.414538
6	0.502005	-0.697657	1.639278
8	0.253894	-1.146900	2.679482
6	3.206358	-0.233567	1.315872
8	4.081519	-0.393380	2.038674
6	-3.379182	0.141114	-1.217948
8	-4.329329	0.232908	-1.858806
6	1.832010	-1.974461	-0.729842
8	1.992195	-3.054851	-1.093268
41	-1.592713	0.000051	-0.089648
41	1.551368	0.047507	-0.077238

10T-1 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.395863	2.076344	0.668338
8	1.381875	3.179333	1.054845
6	0.215399	0.391457	-1.643411
8	-0.658792	0.550372	-2.451850
6	3.100644	0.818968	-1.372680
8	3.931581	1.227169	-2.083195
6	-2.469947	-0.395149	1.727200
8	-2.983286	-0.622804	2.756428
6	-1.844063	2.074410	0.373387
8	-2.125135	3.173946	0.660157
6	-1.774115	-2.098133	-0.492654
8	-1.990122	-3.238245	-0.641921
6	0.381429	-0.960149	1.450580
8	0.210228	-1.613499	2.418499
6	3.100230	-0.310961	1.407208
8	3.927200	-0.528354	2.199172
6	-3.389591	0.297756	-1.131273
8	-4.386265	0.480130	-1.716565
6	1.969388	-1.899223	-0.867453
8	2.226690	-2.953323	-1.301280
41	-1.568141	0.006036	-0.109786
41	1.558794	0.062020	-0.082159

10T-2 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	-1.513424	0.008413	-0.111932
41	1.600172	0.008659	-0.067675
6	-2.720740	0.061926	1.574171
8	-3.390354	0.100659	2.514761
6	3.091299	0.065472	-1.555474
8	3.856526	0.095693	-2.415573
6	-0.285535	-0.232946	1.627456
8	-0.017360	-0.396709	2.752703
6	1.756605	-2.132614	-0.167869
8	1.895689	-3.271311	-0.248106
6	-1.668835	-2.121374	-0.214463
8	-1.803022	-3.264949	-0.234073
6	0.298793	0.071245	-1.668362
8	-0.600376	0.086939	-2.437745
6	-3.406599	0.062040	-1.179818
8	-4.433588	0.070936	-1.687220
6	1.756509	2.150481	0.008140
8	1.902531	3.291140	0.018686
6	2.904025	-0.063881	1.692805
8	3.594488	-0.102007	2.606824
6	-1.527760	2.148237	-0.058759
8	-1.597438	3.295677	0.006861

10T-2 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	1.534933	0.012879	-0.110134
41	-1.597557	0.026509	-0.060518
6	2.669405	-0.022656	1.633192
8	3.300290	-0.034904	2.621867
6	-1.790342	2.153922	0.186568
8	-1.992052	3.301550	0.284722
6	1.463789	2.131788	0.232930
8	1.529330	3.278007	0.456392
6	-0.292459	0.219084	-1.667703
8	0.590822	0.291011	-2.478339
6	3.392247	0.359741	-1.151043
8	4.425499	0.522578	-1.665858
6	-1.820176	-2.093292	-0.345916
8	-2.017563	-3.231643	-0.524459
6	1.913119	-2.072705	-0.457414
8	2.190183	-3.198998	-0.606753
6	-3.094087	0.206823	-1.528797
8	-3.882952	0.306615	-2.388454
6	-2.937927	-0.182915	1.652566
8	-3.670081	-0.292094	2.553273
6	0.262416	-0.687365	1.510361
8	0.022981	-1.153303	2.573639

10T-3 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.285960	1.699560	2.263266
8	0.240082	1.920407	3.390735
6	-1.661202	0.742612	0.271540
8	-2.813822	0.598013	0.367390
6	-2.139826	-2.623839	-0.050281
8	-3.062222	-3.303889	0.000519
6	-0.395368	-1.492307	2.016927
8	-0.433980	-1.593049	3.162658
6	0.838302	-3.166629	0.060444
8	1.511328	-4.098076	0.164124
6	-0.838302	3.166629	-0.060444
8	-1.511328	4.098076	-0.164124
6	0.395368	1.492307	-2.016927
8	0.433980	1.593049	-3.162658
6	2.139826	2.623839	0.050281
8	3.062222	3.303889	-0.000519
6	1.661202	-0.742612	-0.271540
8	2.813822	-0.598013	-0.367390
6	-0.285960	-1.699560	-2.263266
8	-0.240082	-1.920407	-3.390735
41	-0.319348	-1.439774	-0.125290
41	0.319348	1.439774	0.125290

10T-3 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.035909	1.643824	2.018658
8	-0.038122	1.803679	3.176983
6	-1.760812	0.234577	-0.249654
8	-2.834868	-0.261332	-0.321754
6	-1.270348	-3.212602	0.082244
8	-1.933028	-4.172059	0.057746
6	0.117219	-1.721566	2.267218
8	0.178298	-1.922244	3.417253
6	1.710590	-2.794829	0.001394
8	2.655841	-3.485246	-0.069113
6	-1.710590	2.794829	-0.001394
8	-2.655841	3.485246	0.069113
6	-0.117219	1.721566	-2.267218
8	-0.178298	1.922244	-3.417253
6	1.270348	3.212602	-0.082244
8	1.933028	4.172059	-0.057746
6	1.760812	-0.234577	0.249654
8	2.834868	0.261332	0.321754
6	0.035909	-1.643824	-2.018658
8	0.038122	-1.803679	-3.176983
41	0.072576	-1.507932	0.124882
41	-0.072576	1.507932	-0.124882

10T-4 MPW1PW91 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.903760
41	0.000000	0.000000	-1.813217
6	2.167539	0.000000	-1.796491
8	3.312195	0.000000	-1.851584
6	-2.167539	0.000000	-1.796491
8	-3.312195	0.000000	-1.851584
6	0.000000	1.293008	-3.444021
8	0.000000	1.940118	-4.399950
6	0.000000	-1.293008	-3.444021
8	0.000000	-1.940118	-4.399950
6	2.130277	0.000000	1.925984
8	3.284180	0.000000	1.921025
6	0.000000	1.428033	0.405751
8	0.000000	2.111554	-0.564801
6	-2.130277	0.000000	1.925984
8	-3.284180	0.000000	1.921025
6	0.000000	1.538962	3.453996
8	0.000000	2.361850	4.254378
6	0.000000	-1.538962	3.453996
8	0.000000	-2.361850	4.254378
6	0.000000	-1.428033	0.405751
8	0.000000	-2.111554	-0.564801

10T-4 BP86 Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	1.963310
41	0.000000	0.000000	-1.868069
6	2.157589	0.000000	-1.885976
8	3.321576	0.000000	-1.976701
6	-2.157589	0.000000	-1.885976
8	-3.321576	0.000000	-1.976701
6	0.000000	1.303213	-3.492099
8	0.000000	1.971587	-4.456765
6	0.000000	-1.303213	-3.492099
8	0.000000	-1.971587	-4.456765
6	2.143457	0.000000	2.009894
8	3.313711	0.000000	2.037872
6	0.000000	1.398353	0.410246
8	0.000000	2.066000	-0.593565
6	-2.143457	0.000000	2.009894
8	-3.313711	0.000000	2.037872
6	0.000000	1.537746	3.511952
8	0.000000	2.370006	4.329591
6	0.000000	-1.537746	3.511952
8	0.000000	-2.370006	4.329591
6	0.000000	-1.398353	0.410246
8	0.000000	-2.066000	-0.593565

Table S26. Harmonic vibrational frequencies (cm^{-1}) and infrared intensities (in parentheses, in km/mol) for structure **6D-1** of doublet Nb $(CO)_6$ with D_{3d} symmetry. The IR intensities are doubled for the doubly degenerate modes.

	MPW1PW91	**BP86**
A_{1g}	69(0)	66(0)
	375(0)	370(0)
	413(0)	391(0)
	2196(0)	2065(0)
A_{1u}	58(0)	54(0)
	504(0)	484(0)
A_{2g}	333(0)	317(0)
A_{2u}	64(1)	57(0)
	362(24)	355(15)
	485(70)	461(48)
	2085(1784)	1961(1496)
E_g	70(0)	67(0)
	317(0)	303(0)
	345(0)	344(0)
	445(0)	421(0)
	2082(0)	1959(0)
E_u	44(0)	38(0)
	78(2)	73(2)
	367(102)	361(63)
	443(3)	424(2)
	569(173)	544(126)
	2084(5035)	1961(4086)

Table 27. Cartesian coordinates of **16S-1**.

MPW1PW91

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	0.000000
6	0.000000	1.846095	1.105468
6	1.598765	-0.923047	1.105468
6	-1.598765	0.923047	-1.105468
6	-1.598765	-0.923047	1.105468
6	1.598765	0.923047	-1.105468
6	0.000000	-1.846095	-1.105468
8	2.467145	-1.424407	1.669557
8	0.000000	2.848814	1.669557
8	-2.467145	1.424407	-1.669557
8	2.467145	1.424407	-1.669557
8	-2.467145	-1.424407	1.669557
8	0.000000	-2.848814	-1.669557

BP86

Atomic Number	Coordinates (Angstroms) X	Y	Z
41	0.000000	0.000000	0.000000
6	0.000000	1.848330	1.111175
6	1.600701	-0.924165	1.111175
6	-1.600701	0.924165	-1.111175
6	-1.600701	-0.924165	1.111175
6	1.600701	0.924165	-1.111175
6	0.000000	-1.848330	-1.111175
8	2.481347	-1.432607	1.687744
8	0.000000	2.865213	1.687744
8	-2.481347	1.432607	-1.687744
8	2.481347	1.432607	-1.687744
8	-2.481347	-1.432607	1.687744
8	0.000000	-2.865213	-1.687744