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Analogies between Binuclear Phospholyl and Cyclopentadienyl Manganese Carbonyl Complexes: Seven-Electron Donor Bridging Phospholyl Rings

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Supporting Information

Table S1-S5. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structures of $(C_4H_4P)_2Mn_2(CO)_5$.

Table S6-S12. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structures of $(C_4H_4P)_2Mn_2(CO)_4$.

Table S13-S19. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structures of $(C_4H_4P)_2Mn_2(CO)_3$.

Table S20-S24. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structures of $(C_4H_4P)_2Mn_2(CO)_2$.

Table S25. Cartesian coordinates for the 24 structures discussed in this paper.

Table S1. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 5s-1 of $(C_4H_4P)_2Mn_2(CO)_5$ with C_1 symmetry.

	B3LYP			BP86	
a	9	(0)	a	12	(0)
	19	(1)		23	(1)
	32	(1)		32	(1)
	38	(0)		42	(1)
	63	(0)		64	(0)
	78	(0)		77	(0)
	86	(0)		84	(0)
	89	(0)		87	(0)
	97	(0)		95	(0)
	102	(1)		101	(0)
	109	(0)		107	(0)
	117	(0)		116	(0)
	124	(0)		122	(0)
	173	(0)		174	(1)
	184	(1)		187	(1)
	204	(1)		216	(1)
	276	(16)		281	(31)
	282	(1)		290	(3)
	303	(6)		315	(5)
	303	(8)		318	(12)
	328	(12)		340	(7)
	361	(12)		375	(11)
	406	(0)		407	(1)
	441	(1)		427	(3)
	457	(1)		446	(1)
	465	(1)		463	(2)
	479	(2)		482	(8)
	481	(0)		487	(2)
	491	(1)		509	(1)
	512	(23)		520	(2)
	527	(3)		528	(17)
	534	(30)		537	(19)
	542	(31)		545	(10)
	569	(40)		547	(1)
	570	(14)		555	(4)
	578	(2)		572	(7)
	594	(9)		591	(42)
	611	(30)		605	(2)
	625	(79)		620	(154)
	637	(108)		632	(85)
	643	(84)		643	(71)
	654	(64)		647	(62)
	677	(110)		673	(97)
	706	(3)		687	(5)
	721	(3)		697	(4)
	814	(12)		790	(8)

	823	(20)	794	(17)
	842	(11)	808	(9)
	846	(35)	817	(3)
	847	(3)	824	(32)
	854	(15)	826	(11)
	855	(4)	830	(9)
	879	(4)	848	(4)
	913	(2)	867	(3)
	926	(2)	885	(3)
	940	(1)	899	(1)
	946	(1)	901	(1)
	1042	(6)	1012	(6)
	1044	(3)	1016	(3)
	1070	(8)	1033	(8)
	1078	(3)	1043	(2)
	1090	(4)	1055	(3)
	1090	(1)	1055	(1)
	1264	(2)	1212	(2)
	1265	(5)	1213	(6)
	1340	(17)	1294	(21)
	1352	(4)	1306	(6)
	1426	(0)	1382	(2)
	1427	(1)	1384	(1)
	1445	(1)	1393	(1)
	1448	(0)	1394	(0)
	2001	(642)	1926	(493)
	2030	(811)	1946	(775)
	2033	(843)	1950	(692)
	2043	(1324)	1965	(1147)
	2089	(817)	2006	(661)
	3216	(0)	3144	(0)
	3222	(0)	3148	(0)
	3223	(0)	3150	(1)
	3232	(0)	3157	(1)
	3232	(2)	3159	(0)
	3239	(1)	3165	(1)
	3241	(1)	3169	(1)
	3246	(0)	3173	(1)

Table S2. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 5s-2 of $(C_4H_4P)_2Mn_2(CO)_5$ with C_1 symmetry.

	B3LYP			**BP86**	
a	39	(0)	a	38	(0)
	44	(0)		42	(0)
	51	(0)		50	(0)
	67	(0)		67	(0)
	74	(0)		71	(0)
	79	(0)		76	(0)

82	(0)	81	(0)
90	(0)	90	(0)
93	(0)	91	(0)
101	(0)	99	(0)
102	(0)	101	(0)
114	(0)	110	(0)
124	(0)	122	(0)
138	(1)	139	(1)
157	(1)	158	(1)
175	(1)	188	(0)
195	(1)	191	(1)
229	(4)	238	(1)
244	(2)	248	(0)
300	(1)	311	(2)
316	(5)	330	(7)
357	(2)	367	(3)
423	(0)	419	(3)
427	(2)	424	(1)
442	(0)	429	(0)
450	(0)	449	(1)
455	(9)	453	(20)
465	(11)	468	(3)
479	(1)	501	(4)
507	(7)	502	(1)
510	(5)	505	(0)
515	(2)	523	(2)
519	(30)	529	(2)
530	(3)	535	(6)
551	(45)	540	(4)
564	(10)	553	(17)
574	(15)	564	(8)
580	(2)	568	(25)
600	(77)	592	(94)
604	(23)	602	(22)
629	(46)	629	(53)
649	(41)	639	(26)
675	(4)	650	(10)
682	(62)	672	(13)
697	(5)	675	(33)
706	(84)	683	(22)
719	(65)	690	(125)
792	(28)	766	(8)
798	(8)	772	(18)
826	(40)	794	(27)
841	(20)	811	(24)
854	(5)	823	(6)
869	(5)	843	(4)
927	(3)	879	(5)

	931	(2)	884	(2)
	943	(0)	898	(0)
	953	(1)	910	(1)
	1000	(1)	976	(0)
	1043	(1)	1014	(1)
	1080	(3)	1042	(2)
	1092	(2)	1055	(3)
	1099	(9)	1061	(9)
	1103	(17)	1063	(17)
	1263	(3)	1208	(3)
	1282	(1)	1230	(2)
	1346	(1)	1295	(1)
	1371	(2)	1320	(2)
	1428	(1)	1386	(2)
	1459	(3)	1402	(2)
	1479	(51)	1438	(32)
	1584	(0)	1532	(0)
	2002	(204)	1925	(77)
	2026	(926)	1937	(815)
	2033	(630)	1944	(599)
	2048	(1589)	1969	(1296)
	2091	(938)	2006	(727)
	3190	(4)	3116	(5)
	3203	(9)	3129	(10)
	3220	(1)	3144	(1)
	3229	(0)	3156	(0)
	3236	(0)	3166	(2)
	3238	(5)	3168	(0)
	3242	(0)	3171	(2)
	3252	(1)	3173	(2)

Table S3. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 5S-3 of $(C_4H_4P)_2Mn_2(CO)_5$ with C_1 symmetry.

	B3LYP			**BP86**	
a	18	(0)	a	25	(0)
	32	(0)		28	(0)
	48	(1)		50	(1)
	55	(1)		57	(1)
	78	(1)		73	(0)
	88	(0)		86	(0)
	99	(0)		101	(0)
	106	(0)		106	(0)
	113	(0)		112	(0)
	118	(0)		116	(0)
	125	(0)		123	(0)
	133	(0)		133	(0)
	135	(0)		134	(0)
	158	(3)		161	(2)

182	(0)	187	(0)
242	(1)	243	(2)
262	(2)	264	(2)
273	(4)	275	(5)
300	(9)	304	(5)
310	(4)	317	(2)
350	(2)	359	(1)
359	(1)	372	(1)
394	(10)	404	(3)
400	(21)	411	(1)
450	(10)	436	(7)
459	(0)	446	(1)
465	(3)	472	(1)
470	(85)	479	(4)
484	(5)	489	(8)
504	(32)	497	(16)
513	(77)	524	(138)
524	(10)	541	(2)
537	(20)	548	(3)
570	(13)	549	(5)
573	(8)	551	(3)
578	(64)	570	(5)
592	(13)	577	(2)
592	(3)	590	(27)
599	(59)	596	(37)
609	(328)	606	(122)
618	(26)	624	(173)
647	(14)	638	(11)
656	(144)	655	(227)
710	(8)	692	(11)
721	(2)	696	(1)
823	(8)	799	(7)
836	(11)	805	(8)
840	(7)	811	(13)
850	(3)	820	(3)
851	(48)	821	(36)
858	(50)	825	(1)
859	(1)	830	(38)
864	(7)	837	(11)
910	(2)	871	(3)
935	(2)	895	(3)
951	(1)	906	(1)
957	(1)	912	(0)
1050	(3)	1019	(2)
1055	(2)	1023	(2)
1067	(2)	1034	(1)
1077	(2)	1043	(2)
1092	(1)	1056	(1)

	1092	(0)	1057	(0)
	1267	(3)	1215	(6)
	1267	(6)	1216	(4)
	1328	(9)	1290	(8)
	1351	(4)	1307	(6)
	1424	(1)	1376	(1)
	1432	(2)	1388	(1)
	1443	(2)	1391	(1)
	1446	(2)	1400	(1)
	1857	(400)	1775	(331)
	2005	(213)	1917	(185)
	2028	(773)	1941	(664)
	2037	(1553)	1953	(1251)
	2067	(230)	1982	(173)
	3215	(0)	3142	(0)
	3220	(0)	3145	(0)
	3223	(0)	3149	(0)
	3229	(0)	3154	(0)
	3230	(1)	3158	(1)
	3235	(1)	3160	(1)
	3240	(0)	3166	(1)
	3245	(0)	3170	(0)

Table S4. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 5S-4 of $(C_4H_4P)_2Mn_2(CO)_5$ with C_1 symmetry.

	B3LYP			**BP86**	
a	21	(0)	a	22	(0)
	25	(0)		30	(0)
	49	(1)		49	(1)
	52	(1)		59	(1)
	78	(2)		72	(0)
	89	(0)		87	(0)
	99	(0)		102	(0)
	101	(0)		105	(0)
	114	(1)		114	(0)
	117	(0)		115	(0)
	125	(1)		122	(0)
	125	(0)		128	(0)
	135	(0)		137	(0)
	159	(1)		162	(1)
	180	(0)		189	(0)
	251	(5)		245	(0)
	255	(2)		259	(3)
	266	(2)		271	(1)
	286	(4)		298	(10)
	301	(12)		305	(2)
	347	(3)		363	(1)

354	(0)	374	(0)
384	(17)	397	(10)
390	(62)	409	(3)
452	(15)	438	(2)
456	(2)	445	(1)
463	(37)	468	(13)
472	(42)	477	(5)
482	(5)	490	(5)
505	(13)	498	(13)
516	(84)	525	(137)
521	(23)	539	(1)
530	(15)	544	(2)
569	(13)	549	(3)
573	(11)	550	(3)
575	(101)	573	(7)
587	(92)	576	(2)
593	(50)	592	(85)
598	(173)	594	(20)
601	(32)	604	(168)
614	(13)	618	(125)
648	(11)	642	(20)
654	(116)	651	(161)
710	(3)	692	(12)
710	(4)	694	(3)
824	(12)	799	(7)
824	(8)	804	(10)
847	(15)	816	(12)
851	(9)	820	(2)
852	(19)	822	(11)
857	(33)	830	(39)
861	(20)	833	(23)
866	(20)	838	(8)
932	(2)	887	(4)
936	(3)	894	(3)
952	(2)	905	(1)
955	(0)	908	(1)
1048	(3)	1018	(2)
1052	(3)	1021	(2)
1077	(3)	1040	(2)
1079	(2)	1044	(2)
1093	(1)	1055	(0)
1094	(1)	1057	(0)
1268	(4)	1215	(5)
1269	(6)	1217	(5)
1349	(4)	1302	(6)
1353	(5)	1307	(5)
1431	(1)	1384	(1)
1434	(3)	1389	(2)

	1444	(1)	1391	(1)
	1447	(1)	1394	(1)
	1876	(370)	1783	(305)
	1999	(196)	1913	(157)
	2025	(897)	1939	(750)
	2037	(1473)	1953	(1176)
	2065	(238)	1981	(210)
	3215	(1)	3141	(0)
	3217	(0)	3142	(0)
	3223	(0)	3149	(0)
	3225	(0)	3150	(0)
	3230	(1)	3157	(1)
	3232	(1)	3159	(1)
	3241	(0)	3166	(0)
	3242	(0)	3167	(0)

Table S5. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 5S-5 of $(C_4H_4P)_2Mn_2(CO)_5$ with C_1 symmetry.

	B3LYP			**BP86**	
a	30	(0)	a	34	(1)
	36	(1)		38	(1)
	42	(1)		49	(0)
	50	(0)		53	(0)
	75	(1)		76	(0)
	88	(1)		88	(0)
	93	(0)		95	(0)
	99	(0)		100	(0)
	107	(0)		108	(0)
	113	(1)		112	(0)
	127	(1)		130	(0)
	133	(1)		135	(1)
	141	(0)		143	(0)
	154	(3)		158	(2)
	170	(1)		176	(0)
	250	(2)		251	(0)
	258	(1)		265	(2)
	289	(6)		301	(9)
	299	(7)		306	(0)
	305	(6)		313	(3)
	323	(4)		330	(3)
	349	(0)		366	(1)
	387	(16)		400	(25)
	403	(68)		408	(4)
	448	(19)		436	(1)
	453	(22)		443	(0)
	459	(5)		460	(4)
	466	(51)		480	(7)
	479	(5)		484	(2)

489	(47)	503	(101)
512	(11)	505	(12)
520	(17)	532	(15)
529	(25)	538	(7)
569	(22)	545	(1)
571	(74)	551	(5)
575	(1)	573	(3)
586	(16)	576	(2)
591	(78)	583	(140)
594	(25)	589	(17)
595	(210)	600	(91)
616	(57)	619	(107)
646	(116)	641	(95)
655	(42)	653	(163)
705	(4)	685	(7)
713	(7)	694	(17)
810	(10)	784	(10)
826	(10)	800	(8)
843	(44)	811	(32)
846	(7)	814	(10)
849	(25)	819	(13)
856	(6)	828	(6)
858	(11)	830	(13)
862	(18)	834	(13)
929	(3)	889	(4)
934	(1)	891	(1)
947	(0)	899	(1)
957	(0)	910	(1)
1048	(3)	1020	(2)
1052	(2)	1023	(2)
1078	(2)	1044	(2)
1082	(2)	1046	(2)
1091	(3)	1055	(2)
1093	(0)	1057	(0)
1267	(8)	1216	(11)
1268	(2)	1217	(1)
1347	(4)	1305	(5)
1354	(6)	1309	(9)
1431	(1)	1388	(2)
1433	(2)	1389	(0)
1445	(1)	1395	(0)
1455	(1)	1401	(1)
1859	(420)	1770	(337)
2000	(362)	1908	(311)
2031	(323)	1947	(303)
2044	(850)	1960	(668)
2083	(1316)	1999	(1080)
3217	(0)	3144	(0)

	3220	(0)	3146	(0)
	3224	(0)	3149	(0)
	3228	(0)	3152	(0)
	3233	(1)	3158	(0)
	3234	(1)	3158	(0)
	3244	(0)	3166	(1)
	3248	(1)	3167	(0)

Table S6. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 4S-1 of $(C_4H_4P)_2Mn_2(CO)_4$ with C_i symmetry.

	B3LYP			**BP86**	
ag	81	(0)	ag	59	(0)
	103	(0)		81	(0)
	106	(0)		102	(0)
	227	(0)		103	(0)
	264	(0)		174	(0)
	341	(0)		188	(0)
	435	(0)		239	(0)
	506	(0)		286	(0)
	587	(0)		348	(0)
	619	(0)		358	(0)
	656	(0)		420	(0)
	823	(0)		460	(0)
	852	(0)		513	(0)
	884	(0)		522	(0)
	1043	(0)		541	(0)
	1091	(0)		569	(0)
	1308	(0)		582	(0)
	1440	(0)		617	(0)
	2051	(0)		650	(0)
	3235	(0)		693	(0)
	3250	(0)		777	(0)
au	26	(1)		792	(0)
	60	(0)		816	(0)
	104	(0)		841	(0)
	169	(0)		845	(0)
	175	(1)		893	(0)
	344	(3)		1008	(0)
	464	(0)		1020	(0)
	516	(0)		1053	(0)
	567	(25)		1204	(0)
	578	(85)		1267	(0)
	726	(1)		1368	(0)
	812	(11)		1387	(0)
	883	(5)		1924	(0)
	938	(3)		1970	(0)
	1057	(15)		3152	(0)
	1261	(4)		3161	(0)

	1414	(1)		3173	(0)
	2005	(1773)		3176	(0)
	3225	(0)	au	26	(2)
	3246	(2)		60	(0)
bg	60	(0)		81	(2)
	93	(1)		91	(1)
	184	(0)		106	(0)
	339	(0)		181	(1)
	458	(0)		233	(9)
	518	(0)		295	(16)
	560	(0)		355	(5)
	576	(0)		364	(7)
	724	(0)		414	(27)
	808	(0)		467	(2)
	878	(0)		512	(2)
	940	(0)		519	(18)
	1056	(0)		542	(1)
	1259	(0)		592	(77)
	1417	(0)		602	(227)
	2002	(0)		612	(55)
	3225	(0)		649	(95)
	3246	(0)		694	(0)
bu	82	(2)		781	(18)
	213	(7)		784	(33)
	280	(4)		820	(25)
	348	(12)		843	(0)
	428	(29)		846	(5)
	503	(39)		890	(2)
	601	(232)		1007	(9)
	620	(19)		1021	(13)
	655	(93)		1053	(3)
	816	(61)		1206	(4)
	853	(20)		1269	(23)
	883	(0)		1364	(2)
	1041	(8)		1388	(1)
	1091	(3)		1925	(1459)
	1308	(19)		1955	(2311)
	1440	(1)		3152	(0)
	2036	(2605)		3161	(1)
	3235	(1)		3174	(2)
	3249	(2)		3176	(2)

Table S7. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 4S-2 of $(C_4H_4P)_2Mn_2(CO)_4$ with C_1 symmetry.

	B3LYP			**BP86**	
a	22	(1)	a	21	(0)
	33	(0)		32	(0)
	40	(1)		40	(1)

73	(1)	74	(2)
86	(0)	83	(0)
89	(2)	92	(1)
98	(0)	98	(0)
108	(1)	103	(1)
114	(0)	116	(0)
128	(0)	124	(0)
150	(0)	147	(0)
155	(0)	156	(0)
165	(1)	176	(1)
181	(0)	193	(0)
246	(2)	249	(4)
259	(0)	263	(0)
301	(3)	301	(4)
315	(0)	316	(3)
340	(3)	358	(2)
350	(0)	373	(2)
391	(4)	376	(3)
420	(0)	416	(2)
456	(5)	441	(2)
460	(0)	443	(4)
481	(6)	478	(14)
493	(0)	481	(0)
505	(9)	508	(1)
510	(8)	526	(2)
542	(23)	543	(22)
548	(37)	548	(31)
558	(81)	550	(1)
567	(8)	556	(7)
574	(5)	563	(75)
576	(8)	565	(4)
592	(2)	577	(20)
593	(0)	582	(5)
627	(7)	614	(9)
638	(47)	633	(29)
708	(1)	683	(1)
711	(0)	690	(1)
823	(21)	797	(14)
824	(14)	799	(11)
836	(15)	809	(12)
841	(22)	816	(11)
851	(19)	827	(10)
859	(3)	827	(7)
859	(12)	831	(26)
860	(29)	840	(19)
917	(3)	878	(3)
926	(3)	891	(3)
948	(1)	901	(1)

	948	(0)	904	(3)
	1048	(4)	1018	(3)
	1049	(4)	1022	(3)
	1074	(3)	1040	(2)
	1077	(2)	1043	(3)
	1089	(1)	1054	(0)
	1091	(1)	1057	(1)
	1266	(5)	1215	(6)
	1268	(4)	1217	(4)
	1344	(6)	1301	(7)
	1350	(5)	1309	(5)
	1427	(1)	1381	(1)
	1427	(1)	1387	(2)
	1442	(1)	1389	(1)
	1442	(1)	1393	(1)
	1950	(24)	1851	(189)
	1965	(1088)	1868	(571)
	2030	(1477)	1932	(1153)
	2043	(25)	1948	(124)
	3214	(0)	3140	(0)
	3215	(0)	3140	(0)
	3223	(0)	3145	(0)
	3223	(0)	3147	(0)
	3231	(1)	3154	(0)
	3231	(1)	3156	(1)
	3238	(0)	3162	(2)
	3238	(1)	3162	(1)

Table S8. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 4S-3 of $(C_4H_4P)_2Mn_2(CO)_4$ with C_1 symmetry.

	B3LYP			**BP86**	
a	21	(0)	a	27	(1)
	28	(1)		31	(1)
	51	(0)		50	(0)
	69	(0)		69	(1)
	82	(0)		74	(0)
	86	(2)		91	(1)
	95	(0)		95	(1)
	97	(0)		96	(1)
	111	(0)		113	(0)
	128	(1)		128	(1)
	135	(0)		137	(0)
	152	(0)		150	(0)
	163	(0)		154	(0)
	173	(0)		183	(0)
	253	(1)		258	(3)
	289	(1)		298	(3)
	309	(1)		311	(1)

316	(1)	323	(4)
320	(1)	330	(3)
341	(1)	360	(1)
379	(3)	381	(3)
431	(3)	422	(3)
448	(6)	437	(4)
454	(2)	440	(0)
479	(4)	476	(4)
484	(6)	484	(2)
496	(1)	502	(1)
506	(9)	514	(2)
540	(44)	531	(17)
545	(53)	547	(7)
547	(31)	551	(75)
566	(25)	553	(20)
574	(5)	559	(21)
583	(3)	567	(3)
592	(2)	574	(11)
593	(1)	583	(2)
628	(16)	617	(17)
635	(35)	627	(27)
709	(4)	686	(3)
711	(1)	688	(1)
816	(45)	787	(39)
823	(20)	797	(18)
826	(8)	798	(1)
838	(17)	808	(11)
838	(5)	810	(6)
851	(18)	824	(3)
856	(8)	825	(2)
857	(11)	830	(27)
916	(0)	874	(1)
917	(5)	882	(6)
940	(1)	894	(0)
948	(0)	900	(1)
1047	(4)	1018	(4)
1057	(4)	1029	(4)
1069	(1)	1034	(1)
1075	(3)	1042	(3)
1086	(2)	1052	(1)
1090	(1)	1055	(0)
1265	(5)	1213	(7)
1266	(5)	1215	(5)
1328	(4)	1285	(6)
1347	(5)	1303	(6)
1426	(1)	1372	(2)
1427	(3)	1380	(1)
1442	(1)	1391	(1)

	1447	(1)	1408	(0)
	1955	(76)	1864	(128)
	1974	(1119)	1876	(671)
	2027	(129)	1936	(164)
	2065	(1486)	1972	(1208)
	3214	(0)	3139	(0)
	3215	(0)	3140	(0)
	3218	(1)	3144	(0)
	3220	(1)	3144	(1)
	3230	(1)	3155	(1)
	3232	(1)	3156	(0)
	3238	(0)	3163	(1)
	3244	(2)	3163	(2)

Table S9. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 4T-1 of $(C_4H_4P)_2Mn_2(CO)_4$ with C_1 symmetry.

	B3LYP			**BP86**	
a	20	(0)	a	38	(0)
	39	(0)		62	(0)
	53	(1)		62	(0)
	66	(0)		72	(1)
	75	(1)		77	(0)
	75	(1)		88	(0)
	94	(0)		95	(0)
	97	(0)		104	(0)
	101	(0)		118	(0)
	110	(0)		125	(0)
	116	(1)		137	(0)
	124	(0)		147	(1)
	160	(0)		188	(3)
	206	(0)		199	(0)
	224	(5)		241	(7)
	252	(1)		276	(0)
	262	(2)		309	(2)
	266	(1)		318	(12)
	307	(6)		339	(1)
	354	(1)		344	(12)
	367	(18)		420	(7)
	386	(14)		421	(1)
	415	(6)		440	(1)
	440	(1)		445	(2)
	448	(6)		470	(1)
	459	(7)		473	(11)
	493	(2)		491	(51)
	500	(24)		494	(3)
	509	(16)		530	(4)
	516	(14)		531	(1)
	543	(39)		542	(15)

554	(10)	543	(6)
565	(6)	555	(51)
580	(16)	556	(15)
583	(10)	572	(0)
592	(20)	573	(41)
607	(56)	625	(68)
652	(53)	629	(20)
695	(3)	659	(1)
703	(5)	664	(1)
795	(37)	763	(1)
807	(5)	768	(0)
810	(2)	789	(34)
818	(33)	791	(14)
820	(17)	803	(0)
838	(21)	803	(40)
855	(7)	820	(3)
858	(2)	822	(6)
907	(3)	874	(3)
917	(2)	875	(2)
938	(1)	907	(0)
949	(1)	908	(2)
1043	(3)	1011	(3)
1048	(1)	1014	(0)
1073	(3)	1039	(2)
1077	(11)	1043	(13)
1090	(8)	1055	(2)
1090	(1)	1056	(0)
1262	(3)	1209	(1)
1266	(3)	1213	(3)
1325	(2)	1294	(11)
1341	(2)	1298	(0)
1428	(8)	1390	(5)
1431	(15)	1392	(1)
1445	(5)	1398	(0)
1451	(1)	1399	(3)
1981	(298)	1910	(342)
2004	(1044)	1925	(597)
2032	(2373)	1940	(2211)
2065	(606)	1975	(508)
3210	(1)	3135	(2)
3215	(1)	3136	(1)
3224	(0)	3148	(2)
3226	(0)	3149	(0)
3232	(0)	3157	(1)
3236	(0)	3159	(1)
3239	(1)	3166	(1)
3241	(1)	3166	(1)

Table S10. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 4T-2 of $(C_4H_4P)_2Mn_2(CO)_4$ with C_2 symmetry.

	B3LYP			**BP86**	
a	23	(0)	a	27	(0)
	34	(1)		31	(0)
	42	(0)		56	(0)
	53	(1)		59	(1)
	82	(0)		81	(0)
	85	(0)		92	(0)
	95	(0)		94	(1)
	98	(1)		99	(0)
	103	(0)		107	(1)
	107	(2)		125	(0)
	127	(0)		138	(1)
	152	(0)		155	(2)
	153	(4)		160	(1)
	169	(1)		195	(3)
	242	(4)		244	(6)
	273	(3)		271	(4)
	278	(2)		290	(7)
	298	(2)		312	(6)
	311	(1)		317	(7)
	328	(0)		325	(3)
	347	(4)		343	(2)
	417	(85)		419	(17)
	434	(1)		423	(23)
	440	(1)		437	(6)
	448	(4)		449	(7)
	460	(1)		451	(4)
	460	(17)		469	(13)
	497	(90)		500	(70)
	509	(20)		513	(8)
	517	(29)		521	(15)
	541	(39)		522	(5)
	562	(47)		541	(10)
	570	(98)		547	(0)
	576	(210)		565	(2)
	585	(33)		571	(12)
	594	(7)		594	(172)
	616	(34)		613	(34)
	618	(98)		622	(145)
	697	(2)		665	(4)
	706	(4)		685	(8)
	800	(58)		778	(8)
	811	(2)		789	(14)
	816	(14)		792	(10)
	821	(6)		794	(26)
	840	(34)		815	(15)

	847	(5)		817	(5)
	851	(5)		826	(19)
	861	(18)		828	(21)
	893	(2)		865	(3)
	927	(2)		881	(1)
	929	(0)		898	(1)
	950	(1)		911	(1)
	1050	(4)		1022	(5)
	1054	(4)		1025	(4)
	1071	(3)		1041	(4)
	1079	(1)		1044	(1)
	1088	(2)		1055	(1)
	1092	(2)		1059	(2)
	1263	(6)		1212	(6)
	1267	(5)		1215	(5)
	1330	(5)		1293	(7)
	1352	(5)		1302	(6)
	1430	(0)		1388	(1)
	1436	(1)		1391	(0)
	1444	(2)		1396	(3)
	1449	(1)		1397	(0)
	1928	(274)		1785	(383)
	1942	(705)		1847	(348)
	2010	(624)		1936	(405)
	2070	(1244)		1979	(1084)
	3205	(1)		3134	(1)
	3213	(0)		3142	(0)
	3216	(0)		3143	(1)
	3220	(0)		3148	(0)
	3223	(3)		3155	(1)
	3230	(1)		3157	(1)
	3232	(3)		3160	(3)
	3239	(2)		3167	(3)

Table S11. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 4T-3 of $(C_4H_4P)_2Mn_2(CO)_4$ with C_1 symmetry.

	B3LYP			**BP86**	
a	19	(0)	a	17	(0)
	27	(1)		35	(1)
	40	(1)		44	(1)
	46	(0)		49	(0)
	83	(0)		78	(0)
	87	(1)		86	(0)
	96	(1)		93	(0)
	98	(0)		100	(0)
	117	(3)		115	(0)
	120	(0)		118	(0)

125	(1)	126	(1)
144	(2)	146	(0)
166	(3)	165	(1)
203	(0)	215	(2)
251	(7)	259	(2)
258	(1)	261	(4)
281	(3)	289	(2)
304	(3)	317	(2)
310	(4)	320	(2)
349	(31)	349	(3)
352	(21)	362	(3)
405	(60)	413	(15)
430	(5)	421	(2)
441	(7)	429	(13)
453	(4)	438	(15)
466	(45)	467	(7)
478	(1)	478	(1)
504	(56)	508	(83)
511	(23)	513	(4)
531	(19)	530	(0)
536	(50)	535	(9)
563	(2)	548	(4)
573	(31)	553	(13)
586	(26)	567	(9)
590	(34)	570	(3)
595	(221)	591	(158)
617	(71)	611	(47)
637	(110)	628	(144)
697	(2)	671	(4)
712	(5)	692	(5)
812	(9)	785	(6)
820	(46)	799	(48)
826	(11)	801	(4)
828	(23)	803	(13)
846	(19)	814	(10)
848	(3)	818	(1)
854	(11)	820	(22)
859	(16)	826	(11)
908	(2)	871	(2)
921	(3)	876	(3)
941	(0)	900	(0)
955	(1)	916	(1)
1052	(4)	1023	(4)
1052	(2)	1023	(3)
1073	(3)	1039	(2)
1074	(2)	1040	(1)
1090	(1)	1056	(0)
1091	(1)	1057	(1)

	1264	(5)	1213	(6)
	1267	(4)	1216	(5)
	1333	(4)	1291	(6)
	1342	(6)	1297	(8)
	1431	(4)	1381	(3)
	1435	(1)	1388	(1)
	1442	(0)	1397	(1)
	1444	(1)	1397	(0)
	1883	(541)	1782	(430)
	1970	(465)	1869	(300)
	2014	(1420)	1928	(1054)
	2044	(330)	1952	(317)
	3209	(0)	3138	(0)
	3216	(1)	3142	(1)
	3217	(0)	3145	(0)
	3224	(0)	3150	(0)
	3227	(1)	3155	(0)
	3232	(0)	3158	(0)
	3234	(1)	3161	(1)
	3240	(0)	3165	(1)

Table S12. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 4T-4 of $(C_4H_4P)_2Mn_2(CO)_4$ with C_1 symmetry.

	B3LYP			**BP86**	
a	12	(1)	a	19	(1)
	25	(0)		29	(0)
	39	(2)		52	(1)
	51	(1)		55	(1)
	82	(2)		74	(2)
	85	(3)		90	(0)
	94	(1)		96	(1)
	100	(0)		98	(0)
	103	(1)		108	(2)
	118	(2)		122	(2)
	125	(0)		125	(1)
	146	(1)		146	(2)
	160	(5)		156	(3)
	187	(1)		197	(3)
	244	(8)		252	(5)
	261	(1)		268	(2)
	281	(7)		289	(11)
	298	(3)		295	(3)
	305	(1)		308	(10)
	349	(10)		320	(1)
	356	(21)		364	(2)
	395	(75)		419	(13)
	427	(6)		425	(14)
	437	(2)		441	(2)

451	(7)	449	(6)
458	(1)	452	(11)
469	(16)	471	(8)
495	(75)	500	(71)
508	(30)	516	(10)
524	(33)	524	(8)
540	(24)	524	(1)
564	(0)	542	(7)
572	(24)	549	(3)
584	(35)	565	(1)
590	(261)	576	(5)
593	(24)	598	(133)
609	(25)	609	(47)
631	(101)	629	(149)
694	(3)	664	(3)
711	(3)	692	(3)
807	(25)	778	(15)
818	(51)	789	(55)
824	(10)	793	(3)
825	(6)	796	(10)
848	(12)	814	(8)
849	(4)	818	(4)
856	(25)	824	(14)
858	(7)	826	(13)
904	(2)	862	(3)
928	(2)	883	(2)
936	(0)	889	(0)
949	(1)	900	(1)
1049	(3)	1016	(2)
1053	(5)	1020	(5)
1073	(5)	1043	(3)
1077	(2)	1045	(2)
1088	(2)	1057	(1)
1091	(1)	1058	(2)
1262	(4)	1212	(6)
1267	(4)	1216	(5)
1331	(5)	1293	(6)
1349	(4)	1307	(5)
1430	(2)	1385	(1)
1437	(2)	1392	(0)
1442	(3)	1394	(1)
1443	(1)	1395	(3)
1888	(453)	1774	(383)
1966	(587)	1861	(372)
2009	(489)	1933	(342)
2063	(1371)	1973	(1173)
3208	(0)	3136	(0)
3216	(0)	3143	(0)

	3219	(0)	3145	(0)
	3223	(0)	3150	(0)
	3227	(1)	3157	(0)
	3232	(0)	3158	(0)
	3235	(2)	3161	(1)
	3239	(0)	3165	(1)

Table S13. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 3S-1 of $(C_4H_4P)_2Mn_2(CO)_3$ with C_1 symmetry.

	B3LYP			**BP86**	
a	25	(1)	a	23	(0)
	37	(0)		35	(0)
	85	(1)		84	(2)
	89	(1)		87	(2)
	113	(1)		110	(1)
	116	(0)		113	(0)
	133	(0)		140	(0)
	137	(1)		147	(0)
	159	(0)		190	(0)
	162	(0)		193	(0)
	193	(0)		205	(2)
	198	(0)		206	(0)
	293	(4)		295	(9)
	304	(1)		312	(4)
	319	(2)		330	(5)
	322	(6)		340	(3)
	366	(8)		374	(16)
	423	(0)		405	(0)
	425	(0)		423	(0)
	446	(1)		431	(2)
	449	(0)		434	(1)
	464	(9)		457	(1)
	469	(2)		459	(1)
	487	(242)		508	(16)
	514	(27)		513	(7)
	515	(12)		534	(193)
	538	(0)		540	(0)
	568	(0)		540	(3)
	569	(0)		546	(0)
	587	(25)		575	(15)
	593	(20)		575	(2)
	597	(12)		580	(1)
	598	(1)		582	(18)
	710	(1)		689	(0)
	710	(1)		691	(1)
	824	(25)		799	(22)
	825	(0)		800	(0)
	851	(6)		818	(2)

	851	(51)	819	(5)
	852	(0)	821	(35)
	852	(7)	821	(2)
	859	(2)	829	(2)
	860	(4)	829	(5)
	923	(6)	877	(7)
	923	(0)	878	(1)
	943	(1)	895	(2)
	943	(2)	895	(1)
	1053	(2)	1025	(8)
	1053	(8)	1025	(2)
	1074	(1)	1040	(1)
	1074	(4)	1040	(4)
	1090	(1)	1055	(1)
	1090	(3)	1055	(2)
	1265	(2)	1215	(3)
	1266	(6)	1215	(7)
	1344	(6)	1301	(7)
	1344	(2)	1301	(2)
	1436	(0)	1386	(1)
	1436	(1)	1386	(2)
	1438	(1)	1395	(0)
	1438	(2)	1395	(0)
	1928	(989)	1830	(793)
	1929	(998)	1832	(795)
	1957	(0)	1861	(0)
	3215	(0)	3140	(0)
	3215	(0)	3140	(0)
	3222	(0)	3146	(0)
	3222	(0)	3146	(0)
	3231	(0)	3155	(0)
	3231	(0)	3155	(0)
	3238	(1)	3161	(1)
	3238	(0)	3162	(0)

Table S14. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 3S-2 of $(C_4H_4P)_2Mn_2(CO)_3$ with C_1 symmetry.

	B3LYP			**BP86**	
a	34	(1)	a	26	(0)
	55	(0)		39	(1)
	61	(1)		74	(1)
	71	(0)		85	(0)
	89	(0)		96	(0)
	96	(1)		101	(0)
	105	(0)		123	(0)
	126	(1)		133	(2)
	153	(1)		155	(0)
	163	(0)		171	(1)

170	(0)	203	(3)
194	(0)	238	(1)
292	(4)	290	(5)
294	(1)	309	(10)
313	(5)	339	(19)
331	(4)	342	(2)
347	(4)	369	(7)
379	(4)	383	(3)
412	(4)	411	(2)
453	(1)	429	(2)
458	(3)	432	(14)
480	(20)	461	(4)
489	(5)	473	(7)
504	(13)	497	(20)
512	(26)	516	(66)
539	(15)	530	(1)
554	(46)	533	(4)
564	(17)	539	(12)
565	(1)	543	(7)
575	(10)	565	(17)
585	(24)	573	(5)
594	(5)	579	(6)
635	(42)	594	(10)
686	(3)	643	(0)
705	(1)	686	(0)
790	(2)	744	(1)
818	(16)	764	(1)
825	(15)	787	(31)
833	(38)	799	(7)
840	(7)	810	(21)
841	(30)	814	(6)
846	(5)	819	(6)
848	(8)	831	(16)
914	(1)	846	(9)
932	(2)	870	(1)
936	(1)	887	(3)
945	(2)	911	(1)
1039	(4)	1002	(3)
1040	(2)	1027	(3)
1074	(5)	1030	(8)
1081	(3)	1041	(2)
1088	(1)	1049	(0)
1092	(2)	1057	(1)
1261	(5)	1186	(6)
1263	(4)	1216	(6)
1348	(4)	1270	(6)
1352	(3)	1299	(6)
1420	(2)	1377	(0)

	1422	(2)		1382	(1)
	1444	(1)		1385	(0)
	1460	(2)		1402	(0)
	1945	(545)		1813	(367)
	1985	(624)		1909	(547)
	2052	(1337)		1943	(1157)
	3214	(0)		3139	(1)
	3215	(1)		3141	(1)
	3219	(0)		3147	(1)
	3222	(0)		3150	(0)
	3229	(0)		3156	(1)
	3231	(0)		3157	(0)
	3237	(1)		3164	(1)
	3240	(1)		3165	(1)

Table S15. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 3T-1 of $(C_4H_4P)_2Mn_2(CO)_3$ with C_s symmetry.

	B3LYP			**BP86**	
a	27	(0)	A'	73	(1)
	56	(2)		84	(1)
	64	(0)		99	(0)
	75	(1)		147	(0)
	93	(0)		214	(13)
	97	(0)		227	(2)
	102	(1)		268	(2)
	112	(1)		285	(5)
	132	(0)		342	(1)
	147	(1)		362	(4)
	184	(3)		412	(11)
	196	(0)		416	(9)
	260	(2)		520	(10)
	266	(1)		530	(17)
	291	(2)		538	(47)
	301	(4)		573	(64)
	303	(6)		589	(85)
	349	(3)		614	(37)
	406	(33)		651	(41)
	434	(4)		758	(46)
	446	(6)		788	(10)
	451	(2)		804	(5)
	499	(11)		818	(15)
	509	(8)		837	(2)
	513	(30)		844	(0)
	541	(14)		989	(4)
	546	(44)		1009	(4)

557	(1)		1045	(3)
563	(12)		1053	(1)
569	(3)		1268	(12)
575	(15)		1282	(8)
599	(37)		1344	(2)
652	(46)		1390	(0)
683	(4)		1906	(1796)
695	(5)		1959	(849)
773	(28)		3153	(0)
787	(5)		3161	(1)
799	(7)		3167	(1)
809	(44)		3176	(1)
820	(26)	A"	23	(1)
842	(25)		53	(0)
852	(2)		74	(0)
854	(4)		108	(0)
888	(1)		145	(0)
927	(1)		181	(1)
933	(2)		288	(3)
948	(1)		340	(4)
1040	(4)		409	(2)
1044	(2)		463	(2)
1071	(7)		514	(1)
1079	(10)		533	(1)
1089	(2)		538	(1)
1090	(2)		585	(35)
1258	(2)		679	(1)
1262	(5)		698	(0)
1314	(1)		748	(0)
1346	(0)		773	(9)
1426	(2)		823	(0)
1429	(2)		838	(2)
1445	(2)		867	(8)
1464	(1)		888	(0)
1979	(1134)		1021	(6)
2007	(1172)		1024	(9)
2047	(1016)		1201	(1)
3208	(0)		1205	(5)
3215	(1)		1360	(1)
3222	(1)		1378	(0)
3226	(0)		1919	(738)
3232	(0)		3147	(1)
3238	(0)		3151	(0)
3239	(2)		3162	(0)

	3242	(1)		3173	(0)

Table S16. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 3T-2 of $(C_4H_4P)_2Mn_2(CO)_3$ with C_1 symmetry.

	B3LYP			**BP86**	
a	35	(0)	a	29	(0)
	48	(0)		52	(1)
	48	(0)		57	(0)
	70	(0)		74	(0)
	85	(0)		92	(0)
	98	(1)		99	(0)
	100	(0)		102	(0)
	107	(1)		111	(0)
	122	(0)		130	(0)
	132	(0)		141	(1)
	143	(1)		147	(1)
	164	(2)		184	(1)
	230	(2)		255	(3)
	271	(1)		290	(4)
	287	(2)		296	(2)
	295	(2)		305	(3)
	315	(3)		335	(1)
	349	(8)		361	(7)
	392	(13)		403	(10)
	440	(4)		423	(2)
	443	(1)		428	(13)
	452	(2)		434	(2)
	476	(9)		485	(11)
	491	(2)		494	(4)
	506	(24)		516	(4)
	518	(10)		526	(9)
	551	(33)		530	(2)
	556	(9)		540	(2)
	559	(14)		546	(7)
	570	(8)		564	(13)
	584	(5)		567	(23)
	592	(44)		578	(61)
	648	(47)		638	(36)
	689	(3)		660	(5)
	692	(5)		667	(3)
	794	(15)		765	(2)
	795	(3)		768	(8)
	802	(42)		774	(41)
	810	(25)		778	(15)

	824	(27)	780	(21)
	832	(24)	795	(29)
	847	(4)	815	(5)
	852	(4)	817	(1)
	895	(1)	851	(2)
	919	(2)	871	(3)
	927	(1)	879	(2)
	945	(1)	893	(1)
	1043	(2)	1012	(2)
	1045	(6)	1015	(6)
	1074	(6)	1040	(6)
	1078	(2)	1041	(0)
	1086	(3)	1051	(2)
	1092	(1)	1055	(1)
	1260	(5)	1204	(6)
	1262	(6)	1210	(6)
	1334	(14)	1292	(5)
	1343	(4)	1298	(13)
	1424	(1)	1379	(1)
	1425	(10)	1384	(6)
	1450	(2)	1398	(1)
	1454	(1)	1400	(1)
	1925	(538)	1867	(395)
	1992	(647)	1902	(516)
	2050	(1325)	1962	(1084)
	3204	(1)	3130	(0)
	3214	(1)	3140	(1)
	3217	(1)	3143	(1)
	3224	(0)	3150	(0)
	3229	(0)	3158	(0)
	3234	(2)	3162	(1)
	3235	(0)	3163	(1)
	3241	(1)	3168	(1)

Table S17. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 3T-3 of $(C_4H_4P)_2Mn_2(CO)_3$ with C_1 symmetry.

B3LYP			**BP86**		
a	27	(1)	a	23	(1)
	48	(1)		51	(1)
	55	(0)		57	(0)
	67	(1)		66	(1)
	84	(1)		89	(0)
	97	(0)		96	(1)
	99	(1)		101	(0)

107	(1)	107	(0)
126	(1)	130	(1)
139	(0)	142	(1)
151	(2)	166	(2)
163	(2)	183	(2)
223	(2)	256	(3)
250	(1)	283	(2)
290	(1)	298	(5)
297	(3)	312	(3)
328	(6)	338	(7)
347	(9)	366	(3)
385	(12)	406	(1)
443	(2)	420	(14)
444	(1)	424	(17)
453	(2)	429	(3)
473	(4)	482	(7)
489	(2)	491	(5)
495	(22)	519	(4)
515	(20)	522	(6)
550	(12)	528	(12)
554	(26)	538	(2)
559	(26)	544	(9)
568	(3)	562	(22)
592	(6)	570	(13)
594	(44)	575	(54)
649	(46)	635	(36)
691	(5)	664	(4)
697	(4)	675	(1)
785	(4)	762	(3)
794	(2)	768	(6)
800	(74)	777	(21)
819	(38)	780	(58)
821	(9)	788	(14)
829	(21)	789	(17)
849	(5)	817	(4)
849	(2)	819	(2)
901	(3)	851	(3)
922	(2)	873	(4)
928	(1)	887	(1)
947	(1)	897	(1)
1031	(5)	1008	(5)
1043	(2)	1012	(2)
1076	(3)	1039	(7)
1078	(5)	1040	(2)

	1088	(2)	1053	(1)
	1090	(1)	1053	(1)
	1260	(5)	1204	(5)
	1264	(6)	1211	(7)
	1342	(3)	1290	(4)
	1348	(10)	1296	(8)
	1410	(6)	1368	(0)
	1425	(3)	1379	(2)
	1451	(2)	1398	(0)
	1455	(1)	1400	(1)
	1914	(590)	1857	(439)
	1992	(650)	1902	(512)
	2048	(1375)	1960	(1144)
	3210	(0)	3138	(0)
	3217	(1)	3143	(1)
	3217	(0)	3144	(0)
	3226	(0)	3152	(0)
	3228	(0)	3156	(0)
	3235	(1)	3162	(1)
	3236	(0)	3164	(1)
	3242	(1)	3169	(1)

Table S18. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 3T-4 of $(C_4H_4P)_2Mn_2(CO)_3$ with C_1 symmetry.

	B3LYP			**BP86**	
a	29	(2)	a	29	(1)
	33	(0)		42	(0)
	47	(0)		55	(0)
	57	(1)		72	(1)
	79	(1)		92	(0)
	87	(0)		97	(0)
	108	(0)		116	(1)
	119	(3)		120	(3)
	128	(0)		131	(0)
	134	(0)		153	(0)
	141	(0)		166	(1)
	165	(1)		182	(1)
	257	(1)		277	(8)
	278	(3)		283	(4)
	283	(2)		299	(2)
	304	(1)		310	(3)
	314	(1)		329	(7)
	338	(1)		368	(4)
	397	(3)		378	(2)

423	(11)	390	(3)
453	(2)	436	(6)
460	(58)	436	(7)
469	(2)	457	(81)
479	(9)	487	(1)
490	(8)	498	(26)
535	(30)	523	(10)
538	(36)	531	(4)
547	(35)	539	(12)
561	(2)	550	(77)
571	(10)	552	(17)
586	(3)	564	(3)
593	(4)	579	(16)
609	(29)	602	(16)
689	(4)	670	(2)
700	(1)	676	(2)
810	(63)	775	(18)
813	(4)	784	(12)
814	(8)	794	(9)
823	(5)	796	(17)
841	(30)	813	(23)
851	(12)	815	(2)
851	(1)	819	(1)
855	(3)	829	(4)
895	(1)	854	(2)
928	(5)	881	(4)
933	(0)	888	(1)
948	(1)	898	(1)
1052	(2)	1018	(5)
1052	(6)	1026	(3)
1068	(4)	1039	(3)
1075	(3)	1041	(3)
1086	(1)	1050	(1)
1090	(3)	1055	(2)
1260	(6)	1208	(8)
1264	(5)	1213	(7)
1313	(4)	1275	(13)
1343	(8)	1298	(6)
1425	(1)	1377	(2)
1428	(1)	1384	(1)
1439	(1)	1387	(0)
1445	(1)	1396	(0)
1938	(1018)	1834	(625)
1958	(594)	1867	(626)

	2017	(397)	1900	(216)
	3207	(1)	3132	(0)
	3217	(0)	3141	(0)
	3218	(0)	3142	(0)
	3221	(1)	3146	(0)
	3226	(0)	3155	(0)
	3231	(0)	3155	(0)
	3234	(1)	3161	(1)
	3241	(0)	3164	(0)

Table S19. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 3T-5 of $(C_4H_4P)_2Mn_2(CO)_3$ with C_1 symmetry.

	B3LYP			**BP86**	
a	28	(1)	a	27	(1)
	35	(0)		34	(1)
	41	(0)		46	(1)
	56	(0)		60	(1)
	77	(0)		91	(1)
	84	(1)		95	(1)
	105	(0)		117	(0)
	114	(1)		125	(2)
	121	(1)		144	(0)
	141	(1)		171	(0)
	144	(0)		192	(2)
	161	(0)		204	(1)
	232	(2)		252	(7)
	267	(0)		284	(6)
	277	(1)		304	(5)
	295	(5)		318	(1)
	310	(2)		339	(1)
	346	(2)		379	(1)
	393	(7)		389	(1)
	434	(6)		410	(3)
	452	(34)		427	(0)
	455	(23)		435	(4)
	466	(11)		452	(7)
	469	(2)		477	(48)
	490	(4)		502	(4)
	527	(21)		515	(17)
	535	(25)		524	(8)
	552	(39)		537	(10)
	561	(3)		542	(9)
	572	(5)		557	(147)
	584	(6)		565	(5)

590	(6)	567	(10)
609	(37)	593	(22)
690	(4)	673	(7)
701	(1)	684	(0)
796	(21)	776	(4)
805	(13)	786	(11)
813	(34)	792	(23)
816	(19)	792	(9)
845	(30)	815	(18)
850	(16)	820	(2)
852	(3)	822	(16)
855	(4)	827	(4)
899	(1)	858	(1)
931	(2)	884	(5)
933	(1)	896	(1)
943	(2)	906	(1)
1043	(4)	1019	(6)
1047	(5)	1023	(4)
1075	(6)	1040	(3)
1079	(3)	1045	(3)
1086	(3)	1053	(1)
1091	(2)	1058	(1)
1262	(6)	1210	(8)
1266	(4)	1217	(5)
1329	(14)	1282	(17)
1353	(4)	1303	(6)
1424	(1)	1384	(4)
1427	(4)	1389	(1)
1445	(3)	1392	(0)
1446	(2)	1396	(1)
1939	(1078)	1803	(832)
1955	(621)	1821	(216)
2011	(359)	1915	(452)
3206	(0)	3129	(0)
3215	(0)	3140	(1)
3216	(0)	3143	(0)
3222	(0)	3146	(0)
3228	(0)	3156	(0)
3232	(0)	3158	(0)
3234	(1)	3161	(1)
3239	(1)	3163	(1)

Table S20. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in

km/mol) for the structure 2T-1 of $(C_4H_4P)_2Mn_2(CO)_2$ with C_2 symmetry.

	B3LYP			**BP86**	
a	47	(0)	a	54	(0)
	67	(0)		65	(0)
	102	(0)		106	(0)
	118	(1)		121	(1)
	150	(0)		150	(0)
	226	(0)		237	(0)
	305	(0)		317	(3)
	316	(8)		323	(7)
	353	(1)		364	(1)
	429	(3)		402	(0)
	466	(1)		461	(1)
	542	(48)		527	(0)
	551	(0)		543	(1)
	561	(0)		554	(46)
	591	(0)		577	(2)
	693	(1)		665	(0)
	791	(3)		754	(2)
	806	(9)		778	(11)
	818	(0)		787	(0)
	857	(1)		821	(0)
	885	(1)		839	(2)
	933	(5)		884	(2)
	1044	(1)		1007	(1)
	1065	(15)		1027	(14)
	1088	(1)		1052	(0)
	1256	(5)		1199	(4)
	1314	(3)		1265	(3)
	1426	(0)		1373	(1)
	1441	(0)		1393	(0)
	2006	(1388)		1921	(1098)
	3204	(1)		3126	(1)
	3228	(0)		3153	(0)
	3237	(0)		3162	(0)
	3242	(1)		3168	(2)
b	73	(0)	b	71	(0)
	100	(0)		98	(0)
	162	(2)		161	(1)
	207	(1)		217	(3)
	310	(1)		322	(4)
	318	(5)		331	(4)
	365	(8)		375	(13)
	421	(6)		402	(5)

	475	(3)	470	(4)
	533	(22)	524	(0)
	559	(5)	549	(15)
	570	(62)	555	(30)
	585	(4)	575	(23)
	690	(2)	660	(2)
	786	(15)	752	(11)
	808	(15)	779	(10)
	819	(45)	788	(44)
	859	(0)	822	(1)
	884	(2)	838	(2)
	934	(1)	885	(2)
	1042	(9)	1005	(9)
	1063	(3)	1024	(3)
	1087	(1)	1051	(0)
	1253	(2)	1195	(1)
	1310	(4)	1261	(3)
	1426	(5)	1372	(1)
	1440	(2)	1392	(1)
	1974	(988)	1895	(721)
	3203	(2)	3126	(2)
	3228	(0)	3153	(1)
	3235	(0)	3160	(1)
	3242	(1)	3168	(1)

Table S 21. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 2T-2 of $(C_4H_4P)_2Mn_2(CO)_2$ with C_1 symmetry.

B3LYP			**BP86**		
a	33	(1)	a	33	(1)
	34	(0)		42	(0)
	48	(1)		55	(0)
	56	(1)		67	(1)
	77	(5)		82	(1)
	91	(0)		87	(0)
	105	(3)		94	(0)
	108	(2)		114	(0)
	137	(2)		152	(5)
	155	(1)		189	(1)
	228	(2)		266	(1)
	232	(13)		294	(5)
	263	(14)		307	(2)
	279	(6)		320	(5)
	296	(4)		330	(5)
	322	(1)		393	(8)

360	(3)	412	(0)
413	(18)	423	(6)
432	(21)	432	(4)
450	(57)	478	(3)
457	(18)	512	(24)
467	(3)	520	(2)
528	(35)	528	(21)
551	(20)	541	(9)
562	(3)	549	(3)
564	(6)	559	(13)
574	(3)	572	(27)
615	(39)	638	(30)
682	(14)	661	(1)
687	(0)	671	(0)
782	(23)	759	(16)
786	(15)	766	(17)
792	(15)	768	(6)
801	(15)	772	(24)
805	(6)	776	(26)
811	(50)	781	(17)
836	(2)	804	(1)
852	(1)	819	(2)
863	(3)	832	(1)
894	(0)	851	(3)
917	(1)	881	(2)
934	(1)	882	(1)
1035	(5)	1005	(6)
1044	(5)	1017	(4)
1066	(9)	1035	(4)
1070	(10)	1036	(5)
1079	(7)	1050	(1)
1088	(1)	1054	(1)
1252	(11)	1198	(6)
1256	(6)	1205	(7)
1299	(32)	1269	(13)
1317	(4)	1278	(4)
1416	(5)	1368	(0)
1424	(15)	1380	(3)
1430	(1)	1387	(1)
1439	(3)	1396	(1)
1945	(985)	1894	(707)
1998	(1930)	1940	(890)
3202	(1)	3127	(1)
3211	(0)	3141	(0)

	3213	(0)		3143	(1)
	3219	(1)		3149	(0)
	3225	(0)		3152	(0)
	3229	(1)		3156	(1)
	3236	(0)		3163	(0)
	3242	(0)		3168	(1)

Table S 22. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 2T-3 of $(C_4H_4P)_2Mn_2(CO)_2$ with C_s symmetry.

	B3LYP			**BP86**	
A'	36	(1)	A'	36	(1)
	49	(2)		54	(2)
	84	(1)		89	(2)
	103	(0)		105	(1)
	183	(0)		187	(0)
	294	(6)		301	(7)
	307	(6)		310	(8)
	417	(3)		416	(0)
	431	(1)		422	(4)
	453	(2)		476	(52)
	485	(0)		489	(0)
	528	(15)		528	(1)
	529	(10)		531	(1)
	563	(1)		538	(7)
	590	(4)		569	(2)
	700	(3)		679	(2)
	816	(2)		790	(2)
	824	(4)		794	(7)
	832	(6)		800	(6)
	852	(1)		821	(3)
	904	(4)		861	(8)
	942	(1)		894	(1)
	1054	(8)		1022	(8)
	1072	(9)		1039	(8)
	1091	(0)		1057	(1)
	1263	(12)		1211	(13)
	1327	(12)		1288	(10)
	1433	(1)		1382	(1)
	1444	(1)		1399	(1)
	1895	(1133)		1803	(855)
	1919	(262)		1823	(185)
	3208	(0)		3136	(0)
	3217	(0)		3140	(0)

	3230	(0)		3155	(0)
	3236	(2)		3161	(2)
A"	11	(0)	A"	31	(0)
	113	(2)		119	(1)
	120	(0)		137	(0)
	167	(0)		185	(0)
	186	(0)		202	(1)
	279	(2)		295	(5)
	316	(8)		339	(2)
	334	(1)		344	(1)
	413	(34)		409	(2)
	431	(2)		434	(1)
	444	(4)		438	(1)
	561	(3)		535	(8)
	588	(1)		565	(0)
	699	(1)		676	(0)
	815	(42)		788	(22)
	824	(13)		793	(2)
	829	(41)		797	(43)
	851	(3)		821	(1)
	904	(0)		860	(0)
	941	(1)		894	(1)
	1054	(2)		1022	(3)
	1072	(0)		1038	(0)
	1091	(0)		1057	(0)
	1263	(0)		1210	(0)
	1327	(2)		1288	(2)
	1432	(1)		1381	(0)
	1444	(1)		1399	(1)
	3208	(0)		3136	(0)
	3217	(0)		3140	(0)
	3230	(0)		3154	(0)
	3236	(0)		3161	(0)

Table S23. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 2S-1 of $(C_4H_4P)_2Mn_2(CO)_2$ with C_1 symmetry.

B3LYP			**BP86**		
a	28	(1)	a	24	(1)
	33	(0)		33	(0)
	53	(1)		49	(2)
	85	(0)		99	(0)
	96	(1)		103	(1)
	104	(0)		128	(0)

110	(0)	135	(0)
144	(0)	140	(0)
174	(0)	186	(2)
192	(0)	210	(0)
297	(4)	279	(1)
322	(3)	297	(9)
327	(6)	311	(8)
336	(1)	338	(8)
351	(3)	373	(5)
379	(2)	392	(1)
435	(1)	403	(1)
449	(1)	424	(4)
452	(1)	438	(1)
494	(10)	461	(0)
509	(52)	477	(35)
537	(39)	494	(2)
553	(0)	524	(5)
562	(8)	531	(0)
565	(13)	537	(12)
570	(10)	568	(4)
580	(1)	570	(4)
592	(4)	581	(17)
684	(1)	675	(1)
702	(2)	682	(1)
789	(11)	777	(16)
810	(36)	789	(11)
813	(10)	791	(8)
825	(10)	795	(9)
833	(13)	800	(5)
839	(15)	801	(15)
848	(4)	818	(0)
851	(1)	824	(0)
905	(4)	849	(3)
911	(5)	858	(3)
925	(2)	873	(1)
933	(1)	876	(0)
1047	(11)	1017	(7)
1048	(5)	1022	(9)
1070	(6)	1032	(3)
1071	(2)	1040	(3)
1084	(2)	1050	(0)
1089	(4)	1051	(2)
1257	(6)	1208	(6)
1259	(5)	1208	(8)

	1332	(7)	1281	(11)
	1339	(4)	1293	(13)
	1418	(6)	1370	(1)
	1427	(0)	1380	(0)
	1433	(0)	1389	(4)
	1449	(2)	1393	(0)
	1934	(810)	1820	(920)
	1978	(738)	1838	(198)
	3198	(1)	3130	(0)
	3206	(0)	3135	(0)
	3216	(1)	3143	(0)
	3216	(0)	3145	(0)
	3223	(2)	3152	(0)
	3227	(0)	3156	(0)
	3233	(2)	3158	(1)
	3237	(0)	3160	(1)

Table S24. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure 2S-2 of $(C_4H_4P)_2Mn_2(CO)_2$ with C_1 symmetry.

	B3LYP			**BP86**	
a	27	(1)	a	22	(1)
	38	(0)		34	(0)
	40	(0)		49	(1)
	89	(1)		99	(1)
	101	(1)		102	(1)
	132	(0)		133	(0)
	139	(2)		140	(0)
	154	(0)		156	(0)
	182	(0)		186	(0)
	189	(1)		197	(1)
	291	(2)		281	(2)
	307	(2)		289	(3)
	321	(5)		324	(8)
	330	(5)		342	(5)
	367	(6)		376	(3)
	396	(1)		389	(5)
	421	(1)		410	(2)
	449	(4)		417	(3)
	452	(3)		431	(2)
	483	(29)		467	(35)
	498	(15)		474	(6)
	527	(12)		505	(1)
	538	(27)		533	(1)

556	(25)	540	(3)
567	(4)	543	(14)
570	(1)	561	(11)
589	(3)	567	(3)
594	(1)	577	(6)
701	(2)	678	(2)
705	(1)	685	(2)
814	(33)	784	(4)
815	(5)	787	(31)
829	(11)	790	(12)
832	(6)	791	(11)
836	(17)	794	(8)
837	(4)	804	(7)
851	(6)	819	(3)
855	(12)	822	(4)
904	(2)	855	(4)
911	(4)	857	(4)
926	(3)	884	(2)
938	(0)	885	(0)
1045	(7)	1016	(8)
1048	(6)	1018	(4)
1067	(3)	1032	(3)
1069	(4)	1036	(4)
1085	(2)	1052	(1)
1090	(1)	1053	(0)
1258	(7)	1206	(5)
1260	(5)	1207	(8)
1335	(9)	1286	(10)
1336	(1)	1288	(5)
1416	(2)	1368	(1)
1426	(0)	1378	(1)
1433	(0)	1389	(2)
1443	(2)	1390	(0)
1938	(896)	1836	(846)
1957	(493)	1855	(257)
3206	(1)	3138	(1)
3209	(0)	3139	(0)
3218	(0)	3143	(0)
3219	(0)	3148	(0)
3223	(1)	3154	(0)
3227	(1)	3157	(0)
3236	(1)	3164	(1)
3238	(0)	3165	(1)

Table S25. Cartesian coordinates for the 24 structures discussed in this paper.

$(C_4H_4P)_2Mn_2(CO)_5$

5S-1(C_1) / B3LYP

C	1.51689800	1.95582100	0.26631000
C	2.28661000	1.55952200	1.37736000
C	3.57100300	1.04756700	0.98034700
C	3.73624600	1.07886400	-0.42371700
P	2.34751500	1.77816400	-1.30722400
H	1.94516800	1.61082700	2.40791800
H	0.49712100	2.31679600	0.36673400
H	4.63073800	0.70380400	-0.91400400
H	4.31834500	0.67728800	1.67685000
C	-1.11226100	-0.46834200	-1.81631200
C	-2.29069100	-1.25767000	-1.78056200
C	-2.34526100	-2.08163700	-0.60678100
C	-1.22428500	-1.90741200	0.23536200
P	-0.04806100	-0.76486700	-0.44229800
H	-3.06011100	-1.23935200	-2.54654000
H	-0.89484200	0.24836300	-2.60279000
H	-1.10383600	-2.41533400	1.18768300
H	-3.17175600	-2.74967400	-0.38046300
Mn	2.04260400	-0.21166500	0.09462400
Mn	-2.32326000	0.02287700	-0.01324200
C	-1.91539100	0.58306500	1.65192600
C	2.73193400	-1.47779800	-0.97748700
C	-4.08759900	-0.07819000	0.35447300
C	-2.49512100	1.70993900	-0.62610100
C	2.04025000	-1.31219200	1.50835400
O	-5.22377700	-0.15174800	0.58116600
O	-2.58542200	2.78813400	-1.04853600
O	3.23052500	-2.26666200	-1.67409600
O	-1.62526300	0.92812600	2.72217400
O	2.06515800	-2.01556300	2.43852400

5S-1(C_1) / BP86

C	1.48717200	1.94949700	0.27008700
C	2.27837500	1.56213400	1.38451700
C	3.56529100	1.04849600	0.97324700
C	3.70993800	1.06948100	-0.44679700
P	2.30368200	1.76866700	-1.32613400
H	1.94127900	1.61144400	2.42530900
H	0.45570300	2.30122600	0.37853800
H	4.60265500	0.68625900	-0.95238200
H	4.32657200	0.67494600	1.66596900

C	-1.08255300	-0.42099900	-1.82141800
C	-2.25813600	-1.23617800	-1.80915600
C	-2.31448700	-2.07665000	-0.63819800
C	-1.19294000	-1.89800400	0.22241600
P	-0.00625200	-0.74295800	-0.44600500
H	-3.03034400	-1.21134000	-2.58404300
H	-0.86388700	0.31630100	-2.59980400
H	-1.07254200	-2.41218600	1.18061500
H	-3.14199000	-2.76046000	-0.42305200
Mn	2.03366600	-0.18234000	0.10602800
Mn	-2.29886800	0.00107100	-0.03384400
C	-1.86987200	0.59483800	1.59872500
C	2.72768900	-1.46722600	-0.91866400
C	-4.03116300	-0.13251500	0.40250700
C	-2.56510700	1.65949100	-0.64195800
C	2.00933300	-1.27785200	1.50852500
O	-5.17085800	-0.21423600	0.68460900
O	-2.73248800	2.74786000	-1.06077600
O	3.23270600	-2.29493500	-1.59137100
O	-1.57700100	0.97638600	2.67368500
O	2.01888100	-2.00347100	2.44177200

5S-2 (C_1) / B3LYP

C	-0.92800300	-2.62984900	-0.42803000
C	-2.31833600	-2.39974400	-0.47395300
C	-2.65647300	-1.33465400	-1.37746400
C	-1.53252200	-0.77680300	-2.01164000
P	-0.00050400	-1.61331200	-1.58525700
H	-3.04928000	-2.94425200	0.11684800
H	-0.46718700	-3.37528300	0.21368200
H	-1.60257300	0.04725600	-2.71356600
H	-3.67348400	-0.98410600	-1.53410800
C	-0.55669800	2.49665700	-1.55841600
C	-0.69249400	3.78272500	-1.12062400
C	-0.53429100	3.94648700	0.32558000
C	-0.25775700	2.78749700	0.98990400
P	-0.18431200	1.42153900	-0.16940500
H	-0.89196700	4.62655800	-1.78017000
H	-0.61058200	2.18713600	-2.59780900
H	-0.10399300	2.69729900	2.06151500
H	-0.62686800	4.91671000	0.81169100
Mn	-1.28594300	-0.58902800	0.17878400
Mn	1.43995400	-0.22744000	-0.04435000
C	-0.60454200	-0.97101900	1.80048200

C	2.24569400	0.63179200	1.32813200
C	2.68961800	0.37190000	-1.19135400
C	-2.64658900	0.26885900	0.99225000
O	2.76739600	1.16077200	2.21874400
O	3.46994000	0.76444800	-1.95588400
O	-0.27216000	-1.29225000	2.87090800
O	-3.53629200	0.80473100	1.51233700
C	2.32098200	-1.77250500	0.37304500
O	2.91816300	-2.72408700	0.66558600

5S-2 (C_1) / BP86

C	-0.85957700	-2.62252000	-0.40589600
C	-2.26931300	-2.43455000	-0.45056600
C	-2.64228300	-1.37397700	-1.35537600
C	-1.52774800	-0.77739800	-1.99989800
P	0.04327300	-1.57708400	-1.57707600
H	-2.98659900	-2.99865400	0.15391000
H	-0.36484800	-3.35231600	0.24237200
H	-1.62342000	0.04989100	-2.70851900
H	-3.67651600	-1.04526900	-1.50531100
C	-0.56615000	2.48205200	-1.57224800
C	-0.71069900	3.77316000	-1.12177800
C	-0.58745800	3.92568300	0.33381400
C	-0.32368800	2.75530400	1.00258900
P	-0.21619600	1.39889400	-0.17482400
H	-0.88937200	4.62977100	-1.78473600
H	-0.58119900	2.17556400	-2.62230600
H	-0.19348500	2.64665600	2.08347100
H	-0.69237500	4.89949300	0.82899400
Mn	-1.27538900	-0.60835000	0.16284100
Mn	1.41719500	-0.21467600	-0.06544400
C	-0.61364700	-0.96994200	1.78549400
C	2.21125600	0.63380300	1.29007100
C	2.66654300	0.40514100	-1.16446300
C	-2.61191500	0.23775900	0.99695500
O	2.75217400	1.16564800	2.18981000
O	3.48165000	0.81381100	-1.91067700
O	-0.29042000	-1.27401100	2.87971900
O	-3.49895000	0.77131500	1.55874200
C	2.31599900	-1.73045300	0.35410100
O	2.95162200	-2.67438900	0.65726500

5S-3(C_1) / B3LYP

C	2.45937200	-1.38291200	-0.91435200

C	3.12557200	-0.18663600	-1.26701700
C	3.60219000	0.51204900	-0.10795800
C	3.28527400	-0.17175500	1.08697300
P	2.44215200	-1.72568600	0.83002300
H	3.23571000	0.17570700	-2.28537900
H	1.98762500	-2.02351700	-1.65453300
H	3.52796500	0.22574600	2.06916500
H	4.13085200	1.46088800	-0.14754600
C	-3.56710600	-0.19310200	-0.04437100
C	-3.10733500	0.33727600	-1.28469200
C	-2.25756100	1.46224400	-1.09716100
C	-2.08708700	1.78251400	0.27660600
P	-3.01273000	0.73884800	1.36418900
H	-3.35562400	-0.07492200	-2.25911900
H	-4.20912300	-1.06712000	0.02179300
H	-1.45482000	2.59739600	0.61538700
H	-1.78900500	2.00517200	-1.91288100
C	0.10371300	0.04447500	-1.43964000
C	-0.94020200	-1.29330000	1.34051100
C	0.74171000	0.94884900	1.57285400
C	1.36724400	2.07064400	-0.60972000
C	-1.42585800	-1.88613700	-1.03387200
O	1.35769100	3.16837600	-0.99780300
O	0.16725100	0.05453100	-2.62350800
O	-1.51406500	-2.89110600	-1.61080700
O	0.43180100	1.35128600	2.61936700
O	-0.78212000	-1.95362200	2.28127500
Mn	-1.37526100	-0.33188900	-0.14080900
Mn	1.43130400	0.38797900	-0.00228000

5S-3 (C_1) / BP86

C	2.53712400	-1.24324600	-0.99769300
C	3.23208100	-0.00504000	-1.09509900
C	3.54155000	0.53600600	0.20833200
C	3.07557300	-0.31591500	1.25275500
P	2.29430300	-1.82529900	0.67985100
H	3.46935700	0.49580400	-2.03969700
H	2.16895500	-1.77940400	-1.87816000
H	3.17327500	-0.05636300	2.31253200
H	4.05753900	1.48840300	0.37014500
C	-3.50544600	-0.26380000	-0.03497700
C	-3.06600100	0.19877600	-1.32060200
C	-2.25087300	1.37146400	-1.21209600
C	-2.08387700	1.78518600	0.14527300
P	-2.96868900	0.77800100	1.32134600

H	-3.30345200	-0.29233600	-2.27020200
H	-4.11101400	-1.16669300	0.09640000
H	-1.46114000	2.63912200	0.42904000
H	-1.79507400	1.87745900	-2.06888200
C	0.13594400	0.02846500	-1.45083900
C	-0.92063000	-1.23596300	1.35795200
C	0.64566700	1.01163100	1.50519600
C	1.35003400	2.05219800	-0.61847600
C	-1.30872200	-1.90209700	-0.94631100
O	1.33879300	3.16451500	-1.01682900
O	0.19676100	0.02100100	-2.65247700
O	-1.33826700	-2.95627000	-1.47378900
O	0.30681600	1.48829100	2.53065800
O	-0.77007800	-1.88679400	2.32695500
Mn	-1.33457600	-0.32092700	-0.13936300
Mn	1.40460000	0.39098800	0.00153200

5S-4 (C_1) / B3LYP

C	-3.44494000	-0.18907300	0.73365800
C	-3.53884500	0.66558700	-0.38695700
C	-2.91058600	0.10466400	-1.54565000
C	-2.35554200	-1.16767400	-1.26996700
P	-2.63646300	-1.74606500	0.38508800
H	-4.01500100	1.64262200	-0.37168700
H	-3.82881800	0.08657400	1.71244800
H	-1.79355000	-1.72832100	-2.01232300
H	-2.83736900	0.61062300	-2.50403900
C	3.56550400	-0.01057400	-0.25488200
C	3.26919500	-0.41990800	1.06672000
C	2.39130000	0.50816700	1.72350400
C	2.04703400	1.58760300	0.88630600
P	2.82347800	1.53962400	-0.71830800
H	3.65259800	-1.32534000	1.52956100
H	4.19056100	-0.59861400	-0.92185400
H	1.35998700	2.37074500	1.19355300
H	2.01923000	0.37799300	2.73602800
C	-0.89722700	0.50842400	1.76585400
C	0.05116900	0.35103900	-1.34491400
C	1.58287200	-1.60719900	-1.34164900
C	-1.25280100	2.16833800	-0.12446500
C	0.76140300	-1.69643700	1.02743100
O	-1.18646700	3.32644300	-0.21960100
O	-0.68267300	0.61308900	2.90575700
O	0.50353700	-2.57849800	1.73703800

O	1.75872000	-2.40290800	-2.16972600
O	0.02707200	0.61680600	-2.49622100
Mn	1.39599200	-0.38172000	-0.04416100
Mn	-1.41701600	0.39144600	0.04290900

5S-4 (C_1) / BP86

C	-3.26674300	-0.33890000	0.90911300
C	-3.51196500	0.68271700	-0.05339700
C	-3.03305600	0.30675000	-1.36193600
C	-2.43305300	-0.98476300	-1.34809600
P	-2.49194500	-1.81413200	0.23736800
H	-3.99025200	1.64193200	0.17186200
H	-3.51447900	-0.21965000	1.96956000
H	-1.95907400	-1.41807600	-2.23461500
H	-3.08337000	0.95330500	-2.24432900
C	3.40879100	0.10616700	-0.58084600
C	3.35998200	-0.48258900	0.72334000
C	2.58942500	0.32660600	1.63562300
C	2.08219700	1.49669100	1.00974100
P	2.56585000	1.67696700	-0.70655600
H	3.83886300	-1.42938600	0.99444200
H	3.91812100	-0.37147200	-1.42477100
H	1.43803900	2.21247800	1.52944700
H	2.39502100	0.05707700	2.67942000
C	-0.76637200	0.54521100	1.72306700
C	0.00808400	0.30785800	-1.36243200
C	1.44223700	-1.67647300	-1.24196300
C	-1.18140200	2.14974100	-0.12700300
C	0.75677900	-1.65749400	1.08355600
O	-1.08106400	3.32233000	-0.22379300
O	-0.51703100	0.69571100	2.86850300
O	0.52045500	-2.53930200	1.82743400
O	1.55164400	-2.54826300	-2.02812700
O	-0.00484500	0.52516800	-2.54338000
Mn	1.35242800	-0.38157400	-0.03216200
Mn	-1.37779400	0.39345300	0.04572600

5S-5 (C_1) / B3LYP

C	-3.42875900	-0.62695300	0.77275200
C	-3.66725700	0.40882500	-0.15574600
C	-3.09602100	0.12604400	-1.43805300
C	-2.44528400	-1.13205500	-1.44864900
P	-2.55223300	-2.02583300	0.07587900
H	-4.20018900	1.32640600	0.07961300
H	-3.74787200	-0.56837300	1.80993500

H	-1.91669300	-1.49738700	-2.32398200
H	-3.13729200	0.80062900	-2.28836700
C	2.77104700	-1.28940700	-1.20327300
C	1.54332900	-1.94211300	-0.97190100
C	1.26515500	-2.08594200	0.42804100
C	2.27906200	-1.52589500	1.22843400
P	3.64547800	-0.84908200	0.29539800
H	0.88104600	-2.29063400	-1.75936100
H	3.13214000	-1.05591900	-2.20161400
H	2.21555300	-1.49407800	2.31305600
H	0.36334100	-2.54796700	0.81639500
C	1.45045300	1.23598900	1.31426200
C	2.07374000	1.43910200	-1.07054900
C	-0.12112900	0.38308100	-1.35130100
C	-1.46678600	2.02279000	0.25315800
C	-0.89139100	-0.07183400	1.74858800
O	-1.49377700	3.17855900	0.37014700
O	1.57275000	1.97315600	2.20025200
O	-0.66291100	-0.32381600	2.86287000
O	-0.18008100	0.51824600	-2.52681900
O	2.54455500	2.28922700	-1.70361700
Mn	-1.50330300	0.23109700	0.07427200
Mn	1.43010500	0.07763400	-0.08515500

5S-5 (C_1) / BP86

C	-3.33892500	-0.61353600	0.87481400
C	-3.62347500	0.45555300	-0.02119000
C	-3.13636400	0.18699300	-1.35016800
C	-2.49044600	-1.08298300	-1.42239400
P	-2.51480800	-2.01575900	0.09841300
H	-4.13481100	1.37991600	0.26753900
H	-3.58232400	-0.56996000	1.94170600
H	-2.01019900	-1.43537500	-2.34059500
H	-3.21207000	0.88744500	-2.18810900
C	2.69670600	-1.24854900	-1.25524000
C	1.47806600	-1.93705900	-1.00779800
C	1.23682900	-2.11344800	0.40198900
C	2.26616000	-1.54251700	1.19463900
P	3.61032500	-0.82112300	0.23826300
H	0.79701800	-2.27981600	-1.79324900
H	3.02950200	-0.97856400	-2.26332700
H	2.22320200	-1.52156100	2.28887300
H	0.34032100	-2.59346400	0.80666700
C	1.48514400	1.21108400	1.29296900
C	1.95876900	1.43002400	-1.04031200

C	-0.17272800	0.35742900	-1.36916100
C	-1.40195000	1.99931400	0.25690900
C	-0.77005800	-0.09268500	1.68690700
O	-1.40223000	3.17056000	0.38837600
O	1.66441600	1.97745600	2.16587600
O	-0.53326400	-0.35961000	2.81495800
O	-0.19636600	0.48000500	-2.56630500
O	2.39221800	2.32557200	-1.66707000
Mn	-1.47867500	0.22750500	0.06221000
Mn	1.38235800	0.04669600	-0.07453500

$(C_4H_4P)_2Mn_2(CO)_4$

4S-1 (C_i) / B3LYP

C	1.33375600	1.45745000	1.26176000
C	2.64541300	1.58552900	0.71167900
C	2.64541300	1.58552900	-0.71167900
C	1.33375600	1.45745000	-1.26176000
P	0.10489800	1.44313300	0.00000000
H	3.54541700	1.67616200	1.31273700
H	1.12021700	1.43179300	2.32537600
H	1.12021700	1.43179300	-2.32537600
H	3.54541700	1.67616200	-1.31273700
C	-1.33375600	-1.45745000	-1.26176000
C	-2.64541300	-1.58552900	-0.71167900
C	-2.64541300	-1.58552900	0.71167900
C	-1.33375600	-1.45745000	1.26176000
P	-0.10489800	-1.44313300	0.00000000
H	-3.54541700	-1.67616200	-1.31273700
H	-1.12021700	-1.43179300	-2.32537600
H	-1.12021700	-1.43179300	2.32537600
H	-3.54541700	-1.67616200	1.31273700
Mn	1.84070600	-0.29698500	0.00000000
Mn	-1.84070600	0.29698500	0.00000000
C	-2.64541300	1.24921100	-1.29457900
C	2.64541300	-1.24921100	1.29457900
C	-2.64541300	1.24921100	1.29457900
C	2.64541300	-1.24921100	-1.29457900
O	-3.19429200	1.82085100	2.14888100
O	-3.19429200	1.82085100	-2.14888100
O	3.19429200	-1.82085100	2.14888100
O	3.19429200	-1.82085100	-2.14888100

4S-1 (C_i) / BP86

C	-1.93838700	1.23742800	-0.21595900
C	-2.66637300	0.88927300	-1.40451400

C	-2.58551000	-0.51171000	-1.71064100
C	-1.79538000	-1.24024700	-0.75735300
P	-1.24963600	-0.19827900	0.57735700
H	-3.22202000	1.61196600	-2.00993700
H	-1.86028000	2.25143400	0.18570600
H	-1.59674400	-2.31412500	-0.81189700
H	-3.07278900	-0.97346000	-2.57488100
C	1.93838700	-1.23742800	0.21595900
C	2.66637300	-0.88927300	1.40451400
C	2.58551000	0.51171000	1.71064100
C	1.79538000	1.24024700	0.75735300
P	1.24963600	0.19827900	-0.57735700
H	3.22202000	-1.61196600	2.00993700
H	1.86028000	-2.25143400	-0.18570600
H	1.59674400	2.31412500	0.81189700
H	3.07278900	0.97346000	2.57488100
Mn	-0.62917500	0.34193900	-1.73100800
Mn	0.62917500	-0.34193900	1.73100800
C	0.24158500	-1.85829200	2.58831300
C	-0.24158500	1.85829200	-2.58831300
C	0.09807200	0.62800600	3.13160900
C	-0.09807200	-0.62800600	-3.13160900
O	-0.20999000	1.28209900	4.06593900
O	0.02975900	-2.87114400	3.15837900
O	-0.02975900	2.87114400	-3.15837900
O	0.20999000	-1.28209900	-4.06593900

4S-2 (C_1) / B3LYP

C	-3.01219900	-0.06083600	-1.16953400
C	-3.31378300	-0.84541600	-0.02063400
C	-3.00686500	-0.14203200	1.20098500
C	-2.50929300	1.17225200	0.93921800
P	-2.43800600	1.60538600	-0.78568100
H	-3.70083700	-1.86940200	-0.05667100
H	-3.12359400	-0.44016500	-2.19084300
H	-2.17233200	1.84037700	1.73902900
H	-3.12991900	-0.56817900	2.20239300
C	2.83102000	-0.34785800	1.18621600
C	3.18761100	0.90086300	0.59311700
C	3.15750500	0.81875100	-0.84785600
C	2.81418400	-0.48998000	-1.29176500
P	2.55826300	-1.68737800	0.00776900
H	3.42152300	1.81118100	1.15499500
H	2.75139200	-0.47812600	2.27086800

H	2.64930200	-0.72034300	-2.35036100
H	3.35552400	1.66547900	-1.51397900
Mn	-1.20791700	-0.40536900	0.01973000
Mn	1.19401200	0.39800100	-0.02027700
O	-0.85701200	-3.27729800	0.63065800
O	0.03398300	0.37880500	2.70032300
C	0.80472300	2.13090900	-0.10284100
C	-0.30293700	-0.65073700	-1.50323700
C	-0.96245200	-2.12274200	0.40626100
C	0.26643100	0.30931000	1.53228200
O	0.63504000	3.30047400	-0.09776700
O	0.03411600	-0.88468700	-2.62150400

4S-2 (C_1) / BP86

C	-3.01219900	-0.06083600	-1.16953400
C	-3.31378300	-0.84541600	-0.02063400
C	-3.00686500	-0.14203200	1.20098500
C	-2.50929300	1.17225200	0.93921800
P	-2.43800600	1.60538600	-0.78568100
H	-3.70083700	-1.86940200	-0.05667100
H	-3.12359400	-0.44016500	-2.19084300
H	-2.17233200	1.84037700	1.73902900
H	-3.12991900	-0.56817900	2.20239300
C	2.83102000	-0.34785800	1.18621600
C	3.18761100	0.90086300	0.59311700
C	3.15750500	0.81875100	-0.84785600
C	2.81418400	-0.48998000	-1.29176500
P	2.55826300	-1.68737800	0.00776900
H	3.42152300	1.81118100	1.15499500
H	2.75139200	-0.47812600	2.27086800
H	2.64930200	-0.72034300	-2.35036100
H	3.35552400	1.66547900	-1.51397900
Mn	-1.20791700	-0.40536900	0.01973000
Mn	1.19401200	0.39800100	-0.02027700
O	-0.85701200	-3.27729800	0.63065800
O	0.03398300	0.37880500	2.70032300
C	0.80472300	2.13090900	-0.10284100
C	-0.30293700	-0.65073700	-1.50323700
C	-0.96245200	-2.12274200	0.40626100
C	0.26643100	0.30931000	1.53228200
O	0.63504000	3.30047400	-0.09776700
O	0.03411600	-0.88468700	-2.62150400

4S-3 (C_1) / B3LYP

C	2.89813000	-0.71304300	1.15186700

C	1.87853900	-1.71431000	1.09566800
C	1.55603100	-2.09566100	-0.24031800
C	2.33414900	-1.35380900	-1.19064800
P	3.55248000	-0.25988200	-0.46563400
H	1.34933900	-2.09362700	1.97743000
H	3.24280200	-0.26692300	2.09064600
H	2.20222700	-1.45867600	-2.27314500
H	0.79335300	-2.83603500	-0.50006900
C	-2.24478100	-1.29772600	-1.29428100
C	-3.06078100	-0.12886400	-1.19943700
C	-3.45713900	0.12750800	0.16531700
C	-2.91494700	-0.83885100	1.05996500
P	-1.98593800	-2.15398100	0.24715800
H	-3.33490800	0.50571100	-2.04873500
H	-1.78224900	-1.60602500	-2.23903300
H	-3.05814400	-0.78421500	2.14439000
H	-4.07559000	0.97715400	0.47349100
Mn	1.21634600	0.07403600	0.00526500
Mn	-1.31351400	0.22404300	0.01735200
O	-0.19133700	0.33813900	2.76111800
O	0.10504600	0.71334400	-2.66988300
C	-1.50849100	1.99357800	-0.02238100
C	1.64437100	1.78848200	0.26384600
C	-0.47614900	0.30991700	1.60637900
C	0.37376400	0.49388400	-1.53032200
O	-1.71810900	3.15450700	-0.02205400
O	1.98665900	2.90550700	0.41742300

4S-3 (C_1) / BP86

C	2.89813000	-0.71304300	1.15186700
C	1.87853900	-1.71431000	1.09566800
C	1.55603100	-2.09566100	-0.24031800
C	2.33414900	-1.35380900	-1.19064800
P	3.55248000	-0.25988200	-0.46563400
H	1.34933900	-2.09362700	1.97743000
H	3.24280200	-0.26692300	2.09064600
H	2.20222700	-1.45867600	-2.27314500
H	0.79335300	-2.83603500	-0.50006900
C	-2.24478100	-1.29772600	-1.29428100
C	-3.06078100	-0.12886400	-1.19943700
C	-3.45713900	0.12750800	0.16531700
C	-2.91494700	-0.83885100	1.05996500
P	-1.98593800	-2.15398100	0.24715800
H	-3.33490800	0.50571100	-2.04873500

H	-1.78224900	-1.60602500	-2.23903300
H	-3.05814400	-0.78421500	2.14439000
H	-4.07559000	0.97715400	0.47349100
Mn	1.21634600	0.07403600	0.00526500
Mn	-1.31351400	0.22404300	0.01735200
O	-0.19133700	0.33813900	2.76111800
O	0.10504600	0.71334400	-2.66988300
C	-1.50849100	1.99357800	-0.02238100
C	1.64437100	1.78848200	0.26384600
C	-0.47614900	0.30991700	1.60637900
C	0.37376400	0.49388400	-1.53032200
O	-1.71810900	3.15450700	-0.02205400
O	1.98665900	2.90550700	0.41742300

4T-1 (C_1) / B3LYP

C	1.10923300	2.08994100	0.57548500
C	2.37742900	2.19670900	-0.03773700
C	2.35384100	1.72737700	-1.38627000
C	1.06791500	1.30847300	-1.80248000
P	-0.18184600	1.66436100	-0.58702200
H	3.27098400	2.56430200	0.45957200
H	0.91753900	2.37698400	1.60560100
H	0.86853600	0.93558900	-2.80330800
H	3.23159600	1.70037600	-2.02805500
C	-1.32593400	-1.20357700	-1.80359000
C	-2.63211000	-1.43586700	-1.33013300
C	-2.65539200	-1.95931900	0.00612200
C	-1.35062300	-2.12618600	0.52651000
P	-0.06508900	-1.74454400	-0.64717300
H	-3.53110600	-1.21759800	-1.90129300
H	-1.11967100	-0.79966600	-2.79008300
H	-1.15324000	-2.47892200	1.53487800
H	-3.56688800	-2.18723400	0.55147900
Mn	1.73960600	-0.00055600	-0.02606000
Mn	-1.67757400	-0.00635700	0.02654300
C	-3.13033100	1.05269500	-0.13199300
C	2.01380400	-0.55331900	1.67729400
C	-1.55083000	0.42318400	1.76513800
C	3.22793700	-1.08545500	-0.46387100
O	-1.49683600	0.66169700	2.90460500
O	-4.09154000	1.70337900	-0.22340800
O	2.21409400	-0.87695800	2.77959800
O	4.15001400	-1.75389100	-0.67264200

4T-1 (C_1) / BP86

C	1.11834400	2.09714400	0.51335900
C	2.44524300	2.02284700	0.01274600
C	2.48204100	1.49800500	-1.33132600
C	1.19088300	1.18590500	-1.83828900
P	-0.14119600	1.69712600	-0.72101900
H	3.33974100	2.29454400	0.58343400
H	0.87138200	2.42297900	1.52851200
H	1.03301800	0.77601900	-2.84092300
H	3.41078600	1.33853300	-1.89078700
C	-1.19084400	-1.18569400	-1.83843000
C	-2.48201600	-1.49783400	-1.33153200
C	-2.44525400	-2.02283200	0.01248200
C	-1.11836800	-2.09719100	0.51312000
P	0.14120600	-1.69703700	-0.72118100
H	-3.41074600	-1.33828800	-1.89099700
H	-1.03295400	-0.77569300	-2.84101300
H	-0.87143400	-2.42313800	1.52824500
H	-3.33976900	-2.29458500	0.58311700
Mn	1.58034300	0.01353700	-0.02318400
Mn	-1.58033600	-0.01352600	-0.02319800
C	-3.07553900	1.00025400	-0.18390200
C	1.59280300	-0.47616600	1.69416800
C	-1.59283400	0.47594900	1.69422100
C	3.07555100	-1.00022100	-0.18399400
O	-1.64835200	0.76837200	2.83726800
O	-4.05976200	1.64634600	-0.23480900
O	1.64828500	-0.76879300	2.83716600
O	4.05977800	-1.64629700	-0.23497100

4T-2 (C_2) / B3LYP

C	-3.35534500	-0.43212200	-0.96073800
C	-2.40911600	-1.36542700	-1.43672600
C	-1.75078900	-2.04883700	-0.37440600
C	-2.24991000	-1.67165200	0.89902800
P	-3.55775000	-0.47120800	0.83109900
H	-2.14511700	-1.48582700	-2.48500200
H	-3.93707500	0.21028700	-1.61649100
H	-1.85684000	-2.07684800	1.82839000
H	-0.96853100	-2.78680100	-0.53266100
C	2.13704300	-1.78442900	-0.70084200
C	1.78356200	-1.96526600	0.65342600
C	2.52611300	-1.09190300	1.51623800
C	3.42521700	-0.27551200	0.79743200
P	3.43080900	-0.58012700	-0.96384200

H	1.03064600	-2.66356100	1.00803900
H	1.65323000	-2.32300600	-1.51166800
H	4.04312300	0.47795500	1.27878200
H	2.39399200	-1.05333100	2.59437400
Mn	-1.40237200	0.16895000	-0.11483200
Mn	1.36034100	0.13447500	0.11682300
O	0.14559400	0.41899100	-2.58912100
O	-0.23824400	0.54253300	2.59136100
C	1.73398100	1.90111600	0.09363600
C	-1.75767300	1.95097700	-0.16398600
C	0.37474400	0.31176200	-1.44291500
C	0.17995300	0.37980100	1.50823600
O	2.02892000	3.02185700	0.08513700
O	-2.07192300	3.07092900	-0.20646300

4T-2 (C_2) / BP86

C	1.01178200	3.16885600	-0.23694300
C	1.40895700	2.29054200	-1.28083000
C	0.28694100	1.82222100	-2.04464800
C	-0.94948000	2.35897800	-1.56656300
P	-0.76936400	3.51397200	-0.21025200
H	2.44001100	1.95977100	-1.44305500
H	1.72130400	3.59515100	0.47999100
H	-1.92144500	2.08949700	-1.99291500
H	0.37460400	1.12185400	-2.88199500
C	0.94948000	-2.35897800	-1.56656300
C	-0.28694100	-1.82222100	-2.04464800
C	-1.40895700	-2.29054200	-1.28083000
C	-1.01178200	-3.16885600	-0.23694300
P	0.76936400	-3.51397200	-0.21025200
H	-0.37460400	-1.12185400	-2.88199500
H	1.92144500	-2.08949700	-1.99291500
H	-1.72130400	-3.59515100	0.47999100
H	-2.44001100	-1.95977100	-1.44305500
Mn	0.00000000	1.23122400	0.05535400
Mn	0.00000000	-1.23122400	0.05535400
O	2.73309600	-0.09540100	0.27773100
O	-2.73309600	0.09540100	0.27773100
C	-0.06709000	-1.54534100	1.84137300
C	0.06709000	1.54534100	1.84137300
C	1.55318400	-0.27358200	0.19924700
C	-1.55318400	0.27358200	0.19924700
O	-0.09980300	-1.79112500	2.98958400
O	0.09980300	1.79112500	2.98958400

4T-3 (C_1) / B3LYP

C	-3.19445400	0.38980700	-1.08214700
C	-3.51579900	-0.64071700	-0.16939500
C	-3.14555300	-0.31081600	1.17209100
C	-2.55933700	0.98116800	1.24581800
P	-2.49210200	1.83858400	-0.30295000
H	-3.96724300	-1.58792700	-0.45368900
H	-3.36123400	0.29919400	-2.15215300
H	-2.17289000	1.39265200	2.17449300
H	-3.28429600	-0.97241700	2.02256700
C	2.58510000	-1.17844800	-1.01017300
C	2.33736300	-1.73141700	0.27192400
C	2.85843700	-0.91516600	1.31974200
C	3.43693500	0.27472800	0.82933100
P	3.47489700	0.35605600	-0.97273400
H	1.82221300	-2.67433500	0.44013900
H	2.24227400	-1.65134000	-1.92695200
H	3.86161400	1.03931400	1.47445600
H	2.73567900	-1.14573400	2.37525300
Mn	-1.35297000	-0.34973000	-0.07685300
Mn	1.31664400	0.28403100	0.18801900
O	-1.12265500	-3.25511100	-0.59435000
O	-0.06800500	-0.79767300	2.54934800
C	1.11115200	2.08963500	0.32243900
C	-0.34709700	0.05100800	-1.53982500
C	-1.19495200	-2.11285000	-0.39037900
C	-0.20067900	-0.55810200	1.40086100
O	1.06130800	3.24695200	0.43176300
O	0.03728000	0.30464100	-2.61422800

4T-3 (C_1) / BP86

C	-3.19982200	0.35628500	-1.02135400
C	-3.45857100	-0.69595000	-0.09299500
C	-3.04550900	-0.35604900	1.24060900
C	-2.47628100	0.95502600	1.29404700
P	-2.49401100	1.82688700	-0.26589100
H	-3.90060200	-1.66071600	-0.36467200
H	-3.40007800	0.26238300	-2.09388100
H	-2.04865000	1.37379900	2.21129300
H	-3.11793900	-1.03470100	2.09667700
C	2.58748500	-1.08619800	-1.05304700
C	2.35711900	-1.72823300	0.20090800
C	2.81427800	-0.93098100	1.30285500
C	3.34318800	0.32018700	0.87834400

P	3.41046100	0.49733800	-0.93006600
H	1.87291500	-2.70465000	0.31320400
H	2.26071700	-1.51781400	-2.00548600
H	3.71410100	1.08332100	1.57063500
H	2.67124000	-1.21570700	2.35126900
Mn	-1.32387300	-0.33015300	-0.08941700
Mn	1.27952500	0.22620100	0.19635100
O	-1.04122500	-3.16224300	-0.91071400
O	-0.06428500	-1.12976900	2.46639700
C	1.02589600	1.99385600	0.40675300
C	-0.30007400	0.22035600	-1.48343500
C	-1.14146300	-2.03311700	-0.58205500
C	-0.15209800	-0.71768800	1.34085800
O	0.92757300	3.15764800	0.57959600
O	0.07610800	0.55493500	-2.56052400

4T-4 (C_1) / B3LYP

C	2.90234200	-1.06505400	-1.10568900
C	3.54713200	-0.03072800	-0.39357800
C	3.27175300	-0.08930500	1.01326400
C	2.42242900	-1.17830800	1.32942300
P	1.98394200	-2.18902500	-0.06415400
H	4.16225300	0.73654700	-0.85671000
H	2.95674700	-1.15268600	-2.18756600
H	2.06540700	-1.36116600	2.33948900
H	3.65779000	0.62083100	1.73937700
C	-3.35685700	-0.36952100	0.87380200
C	-2.44015200	-1.24873000	1.49218400
C	-1.71548900	-2.02053700	0.53841300
C	-2.13005200	-1.76224900	-0.79170300
P	-3.43947900	-0.56989300	-0.91948700
H	-2.24488400	-1.27492800	2.56204700
H	-3.98228900	0.32352800	1.43030600
H	-1.66654600	-2.24145500	-1.65013300
H	-0.93236400	-2.72652700	0.80144200
Mn	1.40304400	0.21869800	-0.06588300
Mn	-1.35946900	0.17753200	0.12555500
O	1.86742200	3.11317700	-0.49022100
O	0.10214700	0.94784200	2.50577800
C	-1.76478600	1.94726100	-0.00099100
C	0.34664000	0.10279400	-1.55091700
C	1.65689100	1.98426600	-0.32416200
C	0.28147200	0.65308600	1.37796300
O	-2.10711000	3.05710700	-0.07187400

O	-0.03750500	0.00887600	-2.65162100

4T-4 (C_1) / BP86

C	2.81876800	-1.14486000	-1.08642700
C	3.47390400	-0.00946600	-0.53498200
C	3.28611500	0.08237900	0.89681900
C	2.48242100	-0.98591100	1.38709900
P	1.98939400	-2.16835100	0.13253700
H	4.03674700	0.72251400	-1.12415400
H	2.80169300	-1.35354600	-2.16137200
H	2.17785900	-1.05730500	2.43644500
H	3.68766600	0.89032600	1.51730600
C	-3.24458300	-0.34937600	0.93589200
C	-2.31751400	-1.27163800	1.49769900
C	-1.66821200	-2.06030600	0.48900300
C	-2.13619900	-1.75700500	-0.82177500
P	-3.41535600	-0.50694200	-0.87416200
H	-2.06305500	-1.31724300	2.56276400
H	-3.82393500	0.36193000	1.53378600
H	-1.71794400	-2.22420500	-1.71950000
H	-0.88280600	-2.79365400	0.70151800
Mn	1.36702100	0.20276600	-0.09172500
Mn	-1.29942900	0.12832000	0.12005000
O	1.73365900	3.09822500	-0.61321000
O	0.14990700	1.05555700	2.48073900
C	-1.75065000	1.87181500	0.02751000
C	0.29491200	0.02248000	-1.54069300
C	1.56161400	1.95224200	-0.40357400
C	0.20956500	0.70351400	1.33199900
O	-2.11562700	2.99119000	-0.00759000
O	-0.09011900	-0.10744400	-2.66018500

$(C_4H_4P)_2Mn_2(CO)_3$

3S-1 (C_1) / B3LYP

C	-2.80111500	0.70254300	1.14690500
C	-2.64063900	1.56892200	0.03815500
C	-2.73119600	0.86667700	-1.20451500
C	-2.95921700	-0.51733100	-1.01108700
P	-3.11193800	-0.99336500	0.70074000
H	-2.41766900	2.62999600	0.11458500
H	-2.69598900	1.03882200	2.17485100
H	-2.99181000	-1.22733600	-1.83316900
H	-2.58547300	1.33699600	-2.17349000
C	2.95921400	0.51743500	-1.01103600
C	2.73119500	-0.86655300	-1.20460600

C	2.64064100	-1.56892600	0.03799200
C	2.80111600	-0.70266100	1.14683100
P	3.11193600	0.99329500	0.70084000
H	2.58547300	-1.33677300	-2.17362900
H	2.99180600	1.22752500	-1.83304500
H	2.69599100	-1.03904500	2.17474200
H	2.41767400	-2.63000800	0.11431300
Mn	-1.08333100	0.08122500	-0.05481000
Mn	1.08332800	-0.08122100	-0.05481900
C	0.00000000	0.00000000	1.57527100
C	0.21440100	1.40338300	-0.87343800
C	-0.21440000	-1.40331200	-0.87355100
O	-0.24026400	-2.42008500	-1.46665200
O	0.00000000	-0.00010700	2.75190600
O	0.24026100	2.42020200	-1.46645800

3S-1 (C1) / BP86

C	-2.77255300	0.71732300	1.14755800
C	-2.62381700	1.57670400	0.01790300
C	-2.71698700	0.85170500	-1.22033900
C	-2.93588100	-0.54104100	-1.00162100
P	-3.07536600	-0.99950400	0.72766800
H	-2.39510400	2.64632100	0.07828900
H	-2.65159600	1.06610500	2.17867400
H	-2.95580100	-1.27311100	-1.81603600
H	-2.56807600	1.31020700	-2.20404500
C	2.93588000	0.54114600	-1.00156500
C	2.71698000	-0.85157500	-1.22042900
C	2.62381400	-1.57670300	0.01773700
C	2.77255800	-0.71744300	1.14748300
P	3.07537900	0.99942400	0.72776900
H	2.56806600	-1.30997800	-2.20418200
H	2.95580100	1.27330400	-1.81590100
H	2.65160500	-1.06633500	2.17856200
H	2.39509000	-2.64632500	0.07800800
Mn	-1.07971000	0.09080400	-0.05858800
Mn	1.07970900	-0.09079200	-0.05859300
C	0.00000000	0.00000000	1.56328000
C	0.19273500	1.39538600	-0.87404200
C	-0.19274700	-1.39530900	-0.87415200
O	-0.23718200	-2.42711800	-1.47903000
O	0.00000000	-0.00012400	2.75958800
O	0.23718100	2.42724000	-1.47884200

3S-2 (C_1) /B3LYP

C	-1.59341600	-1.87774400	0.86521600
C	-2.85362200	-1.33699600	0.54069200
C	-2.93164900	-0.96903800	-0.85134700
C	-1.75008900	-1.25587400	-1.55113600
P	-0.47338900	-2.03995700	-0.54846000
H	-3.66244500	-1.19157300	1.25119500
H	-1.32480000	-2.18268600	1.87327600
H	-1.60557900	-0.99021900	-2.59511200
H	-3.80126400	-0.49131900	-1.29576800
C	2.69792200	0.69253900	1.06676100
C	2.70610100	1.40762300	-0.15186900
C	2.78741100	0.52151400	-1.28658100
C	2.83401900	-0.83438200	-0.89837600
P	2.85258400	-1.07403200	0.87072900
H	2.63406200	2.48889700	-0.23265500
H	2.57700900	1.17837700	2.03139400
H	2.83427600	-1.65019600	-1.61628100
H	2.77237500	0.86311100	-2.31816900
Mn	-1.28452800	0.12480000	0.13354600
Mn	0.99849800	0.10103800	-0.14749700
C	0.18228000	1.25111500	-1.27408100
C	-2.29786700	1.61932100	0.25268600
C	-0.45887000	0.59760700	1.67701100
O	-0.02111500	2.05848600	-2.10537000
O	-0.14538500	0.88072200	2.76736500
O	-2.94526900	2.57896600	0.34838100

3S-2 (C_1) / BP86

C	1.31487300	-1.48633200	-1.34666900
C	2.68613100	-1.26053200	-1.01595200
C	2.92575800	-1.30241300	0.41011800
C	1.73777900	-1.53575900	1.16102000
P	0.29447800	-1.98852400	0.09757400
H	3.45788900	-0.99759000	-1.74708400
H	0.91899700	-1.48285600	-2.36649500
H	1.70504800	-1.57634100	2.25476000
H	3.89243800	-1.05805200	0.86326400
C	-2.51470000	0.78366600	-1.22571300
C	-2.73700000	1.37436200	0.05923500
C	-2.93974000	0.36922400	1.06282800
C	-2.85368700	-0.95038600	0.53352500
P	-2.59622200	-1.00242400	-1.25001300
H	-2.71553700	2.45112400	0.25630800
H	-2.27890800	1.38569300	-2.10948300
H	-2.91079200	-1.84402500	1.16383500

H	-3.08749100	0.59257200	2.12522600
Mn	1.37318100	0.09797800	-0.05355700
Mn	-0.97107300	0.11270000	0.15298900
C	-0.34722600	0.53243500	1.78715600
C	2.56169100	1.42887600	-0.20237800
C	0.07394000	1.49753100	-0.66990000
O	-0.11781400	0.82274200	2.91268900
O	0.01153500	2.56524000	-1.21033800
O	3.36189300	2.28985700	-0.32224800

3T-1 (C_s) / B3LYP

C	1.47362200	-1.45294100	-1.56147900
C	2.83165000	-1.34020100	-1.20478700
C	3.02803500	-1.31989600	0.20948300
C	1.82551300	-1.51248600	0.93970900
P	0.42121600	-1.81315000	-0.13312000
H	3.64219800	-1.20972500	-1.91845100
H	1.12906700	-1.49221000	-2.59081200
H	1.79105200	-1.55743400	2.02427700
H	4.00039800	-1.18509500	0.67631400
C	-1.48287000	2.02328700	-0.16545300
C	-2.73962900	1.43111300	-0.41397900
C	-2.67735200	0.46137300	-1.47524300
C	-1.38901800	0.32707200	-2.01324900
P	-0.21564100	1.50989400	-1.32824100
H	-3.64469400	1.66118000	0.14090200
H	-1.31471000	2.76255000	0.61253700
H	-1.15135800	-0.37206000	-2.80907100
H	-3.53447000	-0.12593000	-1.79534100
Mn	1.55836200	0.32282200	-0.25424800
Mn	-1.31526100	-0.11712900	0.16514600
C	2.32045900	1.62125500	0.74828200
C	-2.52858800	-1.32377000	0.71841100
O	2.85076100	2.41880300	1.42008900
O	-3.33634100	-2.08351800	1.07256200
C	-0.85850900	0.20019800	1.87569900
O	-0.62673200	0.44411600	2.99025500

3T-1 (C_s) / BP86

C	-1.51284900	1.31703400	1.26896000
C	-1.75593200	2.61550900	0.73022200
C	-1.75593200	2.61550900	-0.73022200
C	-1.51284900	1.31703400	-1.26896000
P	-1.35573900	0.07267400	0.00000000
H	-1.95681500	3.50645000	1.33323300
H	-1.43428700	1.09608700	2.33837800

H	-1.43428700	1.09608700	-2.33837800
H	-1.95681500	3.50645000	-1.33323300
C	1.69823800	-0.97818600	-1.26903900
C	1.94884600	-2.28246100	-0.71758900
C	1.94884600	-2.28246100	0.71758900
C	1.69823800	-0.97818600	1.26903900
P	1.57445700	0.26043000	0.00000000
H	2.12158400	-3.17521400	-1.32647500
H	1.64526300	-0.76318700	-2.33980700
H	1.64526300	-0.76318700	2.33980700
H	2.12158400	-3.17521400	1.32647500
Mn	0.15566000	2.03498300	0.00000000
Mn	0.03604000	-1.68218300	0.00000000
C	1.01583900	3.61507300	0.00000000
C	-0.82613100	-2.58588500	1.27134000
O	1.51537100	4.68951800	0.00000000
O	-1.35430300	-3.21147300	2.12414300
C	-0.82613100	-2.58588500	-1.27134000
O	-1.35430300	-3.21147300	-2.12414300

3T-2 (C_1) / B3LYP

C	1.82288500	-1.30878300	-1.42487700
C	3.01590100	-0.84280900	-0.84816700
C	3.07309600	-1.06148900	0.57128400
C	1.88674800	-1.65518400	1.05780200
P	0.71804100	-2.10196700	-0.24886000
H	3.80311900	-0.34334400	-1.40745500
H	1.58857100	-1.19189900	-2.47904100
H	1.72626600	-1.88344600	2.10787600
H	3.91410500	-0.77432800	1.19597200
C	-2.72321000	0.11006100	1.36123600
C	-2.69113700	-1.24333800	0.93988800
C	-2.99066300	-1.38983900	-0.45411900
C	-3.16085900	-0.15030900	-1.09055700
P	-3.06737400	1.25306900	0.04902400
H	-2.48743400	-2.08406500	1.59959000
H	-2.50156900	0.41420100	2.38095800
H	-3.34080400	-0.04297200	-2.15689000
H	-2.99415200	-2.34953300	-0.96658300
Mn	1.34731000	0.20528400	0.15280500
Mn	-1.06878300	-0.17318500	-0.17687000
C	-0.29847400	0.89100700	-1.44170800
C	2.18929600	1.79430800	-0.06704400
C	0.67103200	0.80302400	1.69642300
O	-0.08372900	1.58647000	-2.36668800

O	0.31557400	1.16912900	2.74729600
O	2.74328400	2.80771500	-0.19013900

3T-2 (C_1) / BP86

C	1.80754800	-1.30361500	-1.41104200
C	2.99456600	-0.77951300	-0.84194400
C	3.06720800	-0.97088900	0.58757600
C	1.88324800	-1.57755500	1.10073700
P	0.70478000	-2.08247500	-0.20237400
H	3.76821300	-0.26188600	-1.41953700
H	1.56033200	-1.21653300	-2.47345500
H	1.72810100	-1.79156700	2.16314500
H	3.90591200	-0.63845700	1.20751700
C	-2.63725100	0.21848300	1.34665300
C	-2.60080200	-1.17358800	1.05234100
C	-2.85154200	-1.44517000	-0.34278200
C	-3.02034500	-0.26117900	-1.10053600
P	-2.95212400	1.25021400	-0.08939900
H	-2.39237600	-1.95605100	1.79137500
H	-2.42646700	0.62280300	2.34221100
H	-3.16943100	-0.25028900	-2.18498300
H	-2.81637700	-2.45250800	-0.77404500
Mn	1.30143900	0.20770900	0.15030000
Mn	-1.02656200	-0.18302400	-0.13469800
C	-0.29131300	0.74637500	-1.49794000
C	2.03674100	1.83294500	-0.05959900
C	0.56284300	0.78468600	1.65731400
O	-0.10492400	1.35858300	-2.50314100
O	0.20270400	1.16471000	2.72272400
O	2.52408500	2.89988200	-0.17087700

3T-3 (C_1) / B3LYP

C	-1.53749000	-1.91696800	0.87536300
C	-2.84122500	-1.45697500	0.58382600
C	-2.96492200	-1.03856000	-0.78516000
C	-1.78439400	-1.22472800	-1.52402900
P	-0.46111400	-1.99203800	-0.57617700
H	-3.64444500	-1.39261000	1.31231800
H	-1.23284400	-2.25594800	1.86155500
H	-1.68257800	-0.93300500	-2.56524300
H	-3.87170200	-0.59912100	-1.19352900
C	2.71018400	0.55034800	1.21764800
C	2.70743900	1.48595300	0.15954600
C	3.02062300	0.86517700	-1.10846800
C	3.23052400	-0.51580500	-0.98855800
P	3.05331700	-1.11335100	0.68668300

H	2.52150200	2.55103900	0.27352000
H	2.46895600	0.81641100	2.24350000
H	3.41608400	-1.16276100	-1.84250500
H	3.06084400	1.41532700	-2.04573500
Mn	-1.36366700	0.11344200	0.21046700
Mn	1.06061800	0.05673100	-0.26817600
C	0.08673500	1.16330600	-1.35414600
C	-0.69818500	0.62082000	1.79070800
C	-2.41302600	1.58910800	0.20883000
O	-0.24187000	1.94398200	-2.17365700
O	-3.09638200	2.52873000	0.22291500
O	-0.34177300	0.92192600	2.86173100

3T-3 (C_1) / BP86

C	-1.50272100	-1.90280400	0.84536100
C	-2.81745500	-1.44416400	0.54307300
C	-2.92774800	-0.99328000	-0.82423100
C	-1.73609700	-1.17803000	-1.56916900
P	-0.39834800	-1.94156300	-0.60971700
H	-3.63090700	-1.38360200	1.27315400
H	-1.19786700	-2.26300800	1.83301800
H	-1.62316300	-0.87013100	-2.61297500
H	-3.83558000	-0.53592800	-1.23277700
C	2.59517300	0.57498900	1.23317900
C	2.60696700	1.49691100	0.13685900
C	2.90194300	0.83967500	-1.12001300
C	3.06565200	-0.55470800	-0.96207900
P	2.91342600	-1.11633100	0.75003500
H	2.42312500	2.57333700	0.22650100
H	2.36268800	0.87342300	2.26072700
H	3.19846700	-1.23727500	-1.80882500
H	2.93102200	1.36298100	-2.08196400
Mn	-1.32009100	0.09987700	0.20057600
Mn	1.01864800	0.08915000	-0.20773600
C	0.08078100	1.08669600	-1.39691500
C	-0.60108000	0.55412500	1.75986000
C	-2.28308900	1.61669900	0.24508200
O	-0.22403600	1.81206200	-2.29397600
O	-2.91616900	2.60943900	0.29461100
O	-0.24877500	0.83428500	2.85828200

3T-4 (C_1) / B3LYP

C	-3.08034100	0.41524100	-1.11768400
C	-2.74803300	-0.95587500	-1.25918100
C	-2.67070000	-1.60918800	0.00101300
C	-3.02494700	-0.74943900	1.08139100

P	-3.50048400	0.88238200	0.57789400
H	-2.48620400	-1.43001600	-2.20219400
H	-3.15186100	1.09813900	-1.96014100
H	-2.99562500	-1.07999900	2.11684300
H	-2.36067200	-2.64427900	0.12820900
C	2.83949600	0.34863300	1.34075900
C	2.41895400	1.56586200	0.74865900
C	2.56113600	1.52801500	-0.67451000
C	3.08001300	0.29796200	-1.13183800
P	3.46406000	-0.85718800	0.18281800
H	2.02052400	2.41498100	1.29642100
H	2.77062100	0.16552100	2.41010600
H	3.21445100	0.07557600	-2.18724500
H	2.24293100	2.33726700	-1.32664000
Mn	-1.21977400	0.10849600	0.04244700
Mn	1.16852100	-0.05205200	-0.05052400
C	0.38138500	-0.86842000	1.36913800
C	0.68659400	-1.28069800	-1.28068900
C	-0.52311300	1.74630300	-0.29858700
O	0.17684800	-1.44541900	2.36981300
O	-0.29206800	2.87115700	-0.54678700
O	0.49657700	-2.09531200	-2.09239500

3T-4 (C_1) / BP86

C	-3.03542100	0.65380700	-0.99147600
C	-2.79555600	-0.72186100	-1.31337900
C	-2.72413800	-1.56331100	-0.15428300
C	-2.88364600	-0.80212200	1.03974800
P	-3.23385800	0.95033200	0.77735600
H	-2.60128300	-1.08445800	-2.33002400
H	-3.09846000	1.44343200	-1.74719400
H	-2.75487000	-1.24011300	2.03627400
H	-2.49334300	-2.63359100	-0.18655700
C	2.85263900	0.33110100	1.30057300
C	2.50740800	1.56517800	0.67018800
C	2.57246000	1.46568200	-0.75897900
C	2.96325800	0.15930700	-1.18026400
P	3.33718300	-0.97554400	0.16452100
H	2.17612200	2.46339900	1.20192300
H	2.80421700	0.18981700	2.38586600
H	3.01107600	-0.12984900	-2.23587600
H	2.29288500	2.27980300	-1.43582500
Mn	-1.18671600	0.03061500	-0.06198700
Mn	1.12270800	0.01449100	-0.00176300
C	0.33049700	-0.93554700	1.32352100

C	0.44643100	-1.13900000	-1.21939600
C	-0.33070600	1.63754200	-0.21582400
O	0.09774700	-1.61231100	2.27451100
O	-0.19686600	2.81935900	-0.35801500
O	0.26094900	-1.94986600	-2.06969000

3T-5 (C_1) / B3LYP

C	-2.95571600	-1.07239600	-0.61964400
C	-2.79966300	-1.28589300	0.77410500
C	-2.98012700	-0.08880900	1.53831400
C	-3.18692500	1.03324100	0.71580500
P	-3.28043800	0.61943800	-1.04367100
H	-2.57618400	-2.25181900	1.22215300
H	-2.83820600	-1.86741000	-1.35160000
H	-3.29401700	2.04474100	1.09841900
H	-2.87899700	-0.05006800	2.62086000
C	2.72798800	1.27384000	-0.68746700
C	2.90141300	0.09264700	-1.44142300
C	3.14231500	-1.04739500	-0.59544800
C	3.13946400	-0.69277600	0.77021800
P	2.89658200	1.06114700	1.06985700
H	2.84602700	0.04163000	-2.52564300
H	2.45692400	2.22199500	-1.14397500
H	3.25866900	-1.42523300	1.56420500
H	3.28445800	-2.05867700	-0.96711400
Mn	-1.18412900	0.13985200	0.15120000
Mn	1.17585200	-0.21929000	-0.14094500
C	-0.36821100	1.70553100	-0.28238100
C	0.46099700	-0.91484300	1.37390500
C	0.43381200	-1.33747200	-1.34259000
O	-0.05516900	2.80235700	-0.55728300
O	0.08053000	-2.09834400	-2.15381000
O	0.30139200	-1.43801700	2.41273700

3T-5 (C_1) / BP86

C	-3.01163800	-0.78989800	-0.87697500
C	-2.88607900	-1.34815300	0.42785700
C	-2.82698300	-0.32096400	1.42976500
C	-2.92654600	0.99624400	0.88804900
P	-3.13121600	1.01315100	-0.90275500
H	-2.77448700	-2.41738600	0.63854000
H	-2.98350500	-1.40337800	-1.78434500
H	-2.86386000	1.90360300	1.49744000
H	-2.63643600	-0.52843400	2.49009000
C	2.64273500	1.26124700	-0.83287200
C	2.51761400	0.12450300	-1.68682900

C	2.80934300	-1.10498100	-0.99688300
C	3.14482900	-0.87544800	0.36431100
P	3.16355900	0.87123200	0.83213700
H	2.18878400	0.17066800	-2.73124000
H	2.40071400	2.27810200	-1.15818700
H	3.33874200	-1.69007600	1.07040500
H	2.72639200	-2.09539100	-1.45672300
Mn	-1.18732200	-0.00979300	0.02188300
Mn	1.11639700	-0.10503900	-0.04601700
C	-0.12309200	1.52787200	-0.10439600
C	0.60738600	-0.69939500	1.57338400
C	0.00867600	-1.37108300	-0.89407800
O	-0.00071700	2.71935200	-0.17085400
O	-0.14770800	-2.34771900	-1.57430300
O	0.41769600	-1.12317300	2.66373900

$(C_4H_4P)_2Mn_2(CO)_2$
2T-1 (C_2) / B3LYP

C	0.29974100	1.71744800	-1.86427600
C	-0.29974100	2.89727200	-1.36443100
C	0.03444800	3.17487700	-0.00542500
C	0.88220300	2.17140400	0.54743500
P	1.38790000	0.94604000	-0.66485500
H	-0.98567200	3.51292000	-1.94343600
H	0.15128700	1.35760200	-2.87779600
H	1.23957600	2.18130400	1.57240500
H	-0.33251400	4.03591300	0.54574300
C	-0.88220300	-2.17140400	0.54743500
C	-0.03444800	-3.17487700	-0.00542500
C	0.29974100	-2.89727200	-1.36443100
C	-0.29974100	-1.71744800	-1.86427600
P	-1.38790000	-0.94604000	-0.66485500
H	0.33251400	-4.03591300	0.54574300
H	-1.23957600	-2.18130400	1.57240500
H	-0.15128700	-1.35760200	-2.87779600
H	0.98567200	-3.51292000	-1.94343600
Mn	-0.89381600	1.20983300	-0.07207200
Mn	0.89381600	-1.20983300	-0.07207200
C	1.62500000	-1.13065700	1.56450000
C	-1.62500000	1.13065700	1.56450000
O	2.05720100	-1.12158900	2.65136100
O	-2.05720100	1.12158900	2.65136100

2T-1 (C_2) / BP86

C	0.24913000	1.71368500	-1.86735400

C	-0.36175200	2.88831800	-1.33819300
C	-0.01448500	3.15175800	0.02983400
C	0.86373700	2.14581400	0.56333500
P	1.38448400	0.94002500	-0.68548700
H	-1.07611500	3.50284200	-1.89984300
H	0.09984900	1.36464600	-2.89358100
H	1.24151800	2.13925400	1.58975500
H	-0.40109100	3.99872000	0.60561300
C	-0.86373700	-2.14581400	0.56333500
C	0.01448500	-3.15175800	0.02983400
C	0.36175200	-2.88831800	-1.33819300
C	-0.24913000	-1.71368500	-1.86735400
P	-1.38448400	-0.94002500	-0.68548700
H	0.40109100	-3.99872000	0.60561300
H	-1.24151800	-2.13925400	1.58975500
H	-0.09984900	-1.36464600	-2.89358100
H	1.07611500	-3.50284200	-1.89984300
Mn	-0.86373700	1.17700900	-0.07746200
Mn	0.86373700	-1.17700900	-0.07746200
C	1.58543300	-1.08855200	1.54754900
C	-1.58543300	1.08855200	1.54754900
O	2.02184900	-1.08070700	2.65073700
O	-2.02184900	1.08070700	2.65073700

2T-2 (C_1) / B3LYP

C	1.70342100	-1.42999600	-1.15446800
C	2.98785100	-0.88466800	-0.89711700
C	3.29052200	-0.80279100	0.49554400
C	2.20559100	-1.19679300	1.30836900
P	0.83727400	-1.89713600	0.33913800
H	3.67640400	-0.56948900	-1.67693200
H	1.30929500	-1.58184200	-2.15482900
H	2.23456400	-1.19433900	2.39424900
H	4.22614700	-0.40312500	0.87943200
C	-2.48703600	0.69709500	-1.15378500
C	-2.63718100	1.30637900	0.13986800
C	-3.04920700	0.36123000	1.12572300
C	-3.14590900	-0.94262800	0.59995300
P	-2.87622600	-1.04645300	-1.17758500
H	-2.48285000	2.36334200	0.34306700
H	-2.20669300	1.26738100	-2.03613700
H	-3.37471000	-1.80822000	1.21824900
H	-3.18416200	0.61159000	2.17602400
Mn	1.44165400	0.41703500	0.07193900
Mn	-0.98461700	-0.15142100	0.15463400

C	1.52265000	1.76561000	-1.15392200
C	0.51929700	1.38585100	1.33071400
O	1.56474900	2.60014900	-1.96545500
O	0.12279600	2.05890800	2.20595200

2T-2 (C_1) / BP86

C	-1.68613500	-1.50645200	1.11010200
C	-2.89750200	-0.76988000	0.93746200
C	-3.20093000	-0.50811500	-0.43943200
C	-2.18516200	-1.00280200	-1.31135400
P	-0.88215400	-1.93506500	-0.44699900
H	-3.51991300	-0.42183600	1.76906700
H	-1.28195200	-1.77949400	2.08948700
H	-2.21100900	-0.87313300	-2.39815000
H	-4.07801100	0.05481100	-0.77489500
C	2.35893900	0.77734500	0.89988800
C	2.55790200	1.15688900	-0.48478100
C	2.87642600	0.02063500	-1.30501200
C	2.87335400	-1.19296600	-0.57714100
P	2.56656600	-1.00169300	1.19703300
H	2.47289400	2.18077200	-0.86570400
H	2.12600000	1.50009200	1.68912300
H	2.98708800	-2.17112100	-1.05813300
H	2.98994400	0.08093000	-2.39458000
Mn	-1.19992400	0.36009800	0.03955000
Mn	0.88461100	-0.10364000	-0.22474100
C	-0.96750700	1.57044200	1.34425300
C	-0.76743900	1.58605900	-1.19245000
O	-0.78946500	2.37243100	2.19406500
O	-0.54054100	2.41281600	-2.01483500

2T-3 (C_s) / B3LYP

C	-0.64549000	1.23329000	2.80153900
C	-1.34053400	-0.00361300	2.90507600
C	-0.45179400	-1.11028800	3.01670100
C	0.90402100	-0.71249700	2.94860500
P	1.12694000	1.06626500	2.86766300
H	-2.42248300	-0.09979100	2.86774900
H	-1.16210800	2.18151200	2.67546200
H	1.73077200	-1.41756900	2.95191700
H	-0.78512000	-2.14549600	3.05147900
C	-0.64549000	1.23329000	-2.80153900
C	-1.34053400	-0.00361300	-2.90507600
C	-0.45179400	-1.11028800	-3.01670100
C	0.90402100	-0.71249700	-2.94860500
P	1.12694000	1.06626500	-2.86766300

H	-2.42248300	-0.09979100	-2.86774900
H	-1.16210800	2.18151200	-2.67546200
H	1.73077200	-1.41756900	-2.95191700
H	-0.78512000	-2.14549600	-3.05147900
Mn	-0.08184100	-0.01373400	1.10210700
Mn	-0.08184100	-0.01373400	-1.10210700
C	-1.68158200	-0.26553900	0.00000000
O	-2.84420700	-0.47822100	0.00000000
C	1.33235500	-0.78977000	0.00000000
O	2.35203800	-1.38295300	0.00000000

2T-3 (C_s) / BP86

C	0.58347600	-1.24287200	2.84769500
C	1.36426700	-0.04284100	2.85375800
C	0.54645400	1.13405800	2.88727700
C	-0.84299200	0.81656400	2.85354600
P	-1.18712300	-0.96081000	2.90166800
H	2.45747300	-0.02023500	2.78942000
H	1.03799400	-2.23712700	2.76975500
H	-1.63249400	1.57339300	2.80058700
H	0.94965900	2.15208800	2.83543200
C	0.58347600	-1.24287200	-2.84769500
C	1.36426700	-0.04284100	-2.85375800
C	0.54645400	1.13405800	-2.88727700
C	-0.84299200	0.81656400	-2.85354600
P	-1.18712300	-0.96081000	-2.90166800
H	2.45747300	-0.02023500	-2.78942000
H	1.03799400	-2.23712700	-2.76975500
H	-1.63249400	1.57339300	-2.80058700
H	0.94965900	2.15208800	-2.83543200
Mn	0.07921000	-0.05757900	1.09797900
Mn	0.07921000	-0.05757900	-1.09797900
C	1.65665300	0.23906400	0.00000000
O	2.83279500	0.48526500	0.00000000
C	-1.29744400	0.75166600	0.00000000
O	-2.32551900	1.37019600	0.00000000

2S-1 (C_1) / B3LYP

C	2.35901400	-1.50586800	0.36129800
C	3.26806500	-0.74615600	-0.39605700
C	3.31153600	0.63374900	-0.01477500
C	2.39482000	0.89584700	1.04095300
P	1.50083700	-0.55599000	1.63192500
H	3.82959700	-1.14992100	-1.23736500
H	2.15752500	-2.55384300	0.15539500
H	2.24553800	1.89033400	1.45395500

H	3.95679800	1.37895500	-0.47054400
C	-2.48791500	1.18589400	0.71100200
C	-2.06554100	0.36476100	1.78580700
C	-2.17423600	-1.02874800	1.47293200
C	-2.69419000	-1.22907700	0.17024400
P	-3.09445400	0.29057000	-0.70262900
H	-1.64192500	0.74105800	2.71412500
H	-2.39270900	2.26910300	0.72735200
H	-2.80506800	-2.21714800	-0.26876900
H	-1.86044300	-1.82831200	2.13875600
Mn	1.27751200	0.18605300	-0.59679200
Mn	-0.84712800	-0.08742500	0.08112400
C	-0.38569000	-1.14576200	-1.29154500
O	-0.35727000	-1.91366100	-2.18734300
C	0.44278500	1.77552100	-0.77775200
O	0.08770100	2.88671100	-0.89181800

2S-1 (C_1) / BP86

C	2.62249000	-1.29298200	0.48847900
C	3.06412700	-0.81230900	-0.78124500
C	3.10797000	0.62301300	-0.82307200
C	2.70111400	1.20308900	0.41747000
P	2.28761900	0.00334000	1.69815200
H	3.26847800	-1.46045800	-1.64115300
H	2.44947800	-2.35720700	0.68197700
H	2.59955900	2.28569800	0.54992800
H	3.35305000	1.20680100	-1.71756000
C	-2.82632200	1.05361100	-0.35251000
C	-2.38433900	1.35647300	0.97946900
C	-2.24432100	0.17069000	1.77843100
C	-2.54477600	-1.01542900	1.03876700
P	-3.10488500	-0.68988200	-0.64716700
H	-2.13428800	2.36445200	1.32839500
H	-2.93164900	1.82388800	-1.12358100
H	-2.43216300	-2.02413600	1.45020400
H	-1.84664200	0.17303900	2.80064400
Mn	1.08229300	-0.01686300	-0.35813300
Mn	-0.93576100	0.06214900	0.08881000
C	-0.10261400	-1.51222400	-0.69035800
O	-0.21151100	-2.65986000	-1.01687800
C	0.02252200	1.49215500	-0.86053800
O	-0.06664400	2.60453100	-1.29935900

2S-2 (C_1) / B3LYP

C	2.98921000	-0.41877600	-0.77915000
C	2.73918900	0.97406500	-0.88861900

C	2.48131900	1.56206800	0.39073100
C	2.52934900	0.60628900	1.43580700
P	2.95429800	-1.03920600	0.90424400
H	2.70883600	1.52296700	-1.82595900
H	3.16025800	-1.05398900	-1.64399500
H	2.28066300	0.85448400	2.46558200
H	2.20759600	2.60529300	0.52536300
C	-2.44517200	0.78795200	1.18494900
C	-1.77516100	-0.36169600	1.69995600
C	-2.11004700	-1.53069200	0.93876900
C	-2.98538000	-1.24799700	-0.12784900
P	-3.51466600	0.45791400	-0.20718400
H	-1.12946600	-0.36233500	2.57333900
H	-2.30329500	1.78246200	1.59993400
H	-3.27223400	-2.00218100	-0.85737800
H	-1.66600800	-2.50748300	1.11616000
Mn	1.01206300	0.05080500	-0.02237200
Mn	-1.13807600	-0.00772000	-0.30362400
C	0.42723000	-1.38324600	-0.96515300
C	-0.42132200	1.62983800	-0.64983300
O	0.40957600	-2.38735100	-1.58174600
O	-0.28529800	2.77437700	-0.88034400

2S-2 (C_1) / BP86

C	2.94364900	-0.57598700	-0.77914500
C	2.80674700	0.82683900	-1.00180200
C	2.55862200	1.54169300	0.22005800
C	2.54284900	0.67119500	1.35687900
P	2.84888200	-1.05448700	0.96361000
H	2.79653200	1.29825400	-1.99093100
H	3.06915000	-1.30413400	-1.58694400
H	2.30501400	1.02631800	2.36621200
H	2.35167500	2.61629700	0.26081800
C	-2.50547200	0.82115200	1.15993300
C	-1.93961600	-0.36564000	1.73763300
C	-2.18542200	-1.51433200	0.90582500
C	-2.93135000	-1.19037800	-0.26639100
P	-3.40375700	0.53438000	-0.37424200
H	-1.37370300	-0.39366100	2.67391900
H	-2.39121600	1.81564100	1.60377500
H	-3.13920600	-1.92715800	-1.05015900
H	-1.77675300	-2.50975400	1.11257000
Mn	1.00665000	0.07420900	-0.02603100
Mn	-1.05358800	-0.01598500	-0.16685400
C	0.23712300	-1.37422500	-0.93266900

C	-0.29483300	1.62137100	-0.55822000
O	0.26536500	-2.42208700	-1.51071700
O	-0.23270200	2.79134900	-0.79681600