Unsaturation and Variable Hapticity in Binuclear Azulene Manganese Carbonyl Complexes

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• Manganese-carbon and carbon-carbon distances (in Å) for the $C_{10}H_8Mn_2(CO)_n$ (n = 6, 5, 4, 3, 2) structures (Tables S1 to S6);

• Complete tables of harmonic vibrational frequencies for the $C_{10}H_8Mn_2(CO)_n$ (n = 6, 5, 4, 3, 2) structures (Tables S7 to S26);

• Optimized coordinates for the the $C_{10}H_8Mn_2(CO)_n$ (n = 6, 5, 4, 3, 2) structures (Table S38)

• Complete Gaussian reference (reference 35).

Table S1. Manganese-carbon and carbon-carbon distances (in Å) for the $C_{10}H_8Mn_2(CO)_6$ structures

	6S-1			6S-2		6T-3		6T-4	
	B3LYP	BP86	Exp.	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
Mn1-C1	2.156	2.151	2.123	2.163	2.154	2.238	2.157	3.925	4.012
Mn1-C2	2.186	2.162	2.131	2.165	2.142	2.124	2.123	4.228	4.368
Mn1-C3	2.353	2.318	2.275	2.296	2.263	2.214	2.234	3.991	4.210
Mn1-C4	3.057	3.049	3.014	3.104	3.089	3.007	2.947	3.308	3.638
Mn1-C8	3.057	3.049	2.992	3.104	3.089	3.536	3.351	2.415	2.982
Mn1-C9	2.353	2.318	2.283	2.296	2.263	3.514	3.158	2.176	2.587
Mn1-C10	2.186	2.162	2.142	2.165	2.142	2.965	2.481	3.131	3.238
Mn2-C4	2.230	2.215	2.186	2.204	2.187	2.235	2.250	2.279	2.209
Mn2-C5	2.189	2.172	2.178	2.177	2.162	2.191	2.180	2.265	2.179
Mn2-C6	2.154	2.142	2.151	2.159	2.142	2.171	2.151	2.262	2.166
Mn2-C7	2.189	2.172	2.152	2.177	2.162	2.171	2.155	2.213	2.157
Mn2-C8	2.229	2.215	2.178	2.204	2.187	2.210	2.249	2.269	2.140
C1-C2	1.429	1.435	1.427	1.431	1.439	1.415	1.433	1.450	1.439
C2-C3	1.405	1.421	1.425	1.413	1.429	1.418	1.429	1.364	1.384
C3-C4	1.475	1.478	1.476	1.481	1.484	1.474	1.463	1.451	1.450
C8-C9	1.475	1.478	1.476	1.481	1.484	1.435	1.429	1.465	1.453
C9-C10	1.405	1.421	1.396	1.413	1.429	1.363	1.423	1.458	1.426
C10-C1	1.429	1.435	1.418	1.431	1.439	1.466	1.437	1.369	1.400
C4-C8	1.429	1.438	1.419	1.410	1.422	1.452	1.465	1.468	1.467
C4-C5	1.420	1.431	1.437	1.437	1.446	1.422	1.440	1.428	1.436
C5-C6	1.436	1.445	1.417	1.430	1.441	1.435	1.443	1.419	1.445
C6-C7	1.436	1.445	1.445	1.430	1.440	1.423	1.430	1.417	1.427
C7-C8	1.420	1.431	1.444	1.437	1.446	1.434	1.453	1.454	1.450

Table S2. Manganese-carbon and carbon-carbon distances (in Å) for the singlet $C_{10}H_8Mn_2(CO)_5$ structures

	5S-1		5S-2		5S-3	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
Mn1-C1	2.117	2.118	2.160	2.143	2.151	2.138
Mn1-C2	2.201	2.179	2.176	2.157	2.196	2.159
Mn1-C3	2.318	2.292	2.311	2.263	2.399	2.338
Mn1-C4	2.574	2.501	2.962	2.893	3.092	3.048
Mn1-C8	2.574	2.501	3.442	3.403	3.045	3.063
Mn1-C9	2.318	2.292	3.000	2.983	2.313	2.363
Mn1-C10	2.201	2.179	2.323	2.284	2.171	2.166
Mn2-C4	2.307	2.337	2.120	2.125	2.173	2.154
Mn2-C5	2.191	2.179	2.189	2.180	2.150	2.154
Mn2-C6	2.144	2.121	2.173	2.162	2.134	2.103
Mn2-C7	2.191	2.178	2.089	2.084	2.189	2.137
Mn2-C8	2.307	2.337	2.003	2.004	2.190	2.149
C1-C2	1.428	1.431	1.432	1.439	1.435	1.435
C2-C3	1.396	1.413	1.408	1.421	1.400	1.426
C3-C4	1.446	1.440	1.450	1.453	1.477	1.471
C8-C9	1.446	1.440	1.429	1.438	1.476	1.472
C9-C10	1.396	1.413	1.445	1.456	1.415	1.422
C10-C1	1.428	1.431	1.413	1.425	1.427	1.437
C4-C8	1.448	1.463	1.470	1.479	1.426	1.446
C4-C5	1.434	1.447	1.429	1.435	1.429	1.427
C5-C6	1.427	1.436	1.434	1.440	1.430	1.449
C6-C7	1.427	1.436	1.420	1.431	1.445	1.447
C7-C8	1.434	1.447	1.451	1.461	1.414	1.431

Table S3. Manganese-carbon and carbon-carbon distances (in Å) for the triplet $C_{10}H_8Mn_2(CO)_5$ structures

	5T-4		5T-5		5T-6	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
Mn1-C1	2.225	2.188	2.216	2.224	2.159	2.154
Mn1-C2	2.175	2.147	2.115	2.112	2.184	2.157
Mn1-C3	2.230	2.212	2.130	2.137	2.351	2.307
Mn1-C4	3.014	2.976	2.450	2.434	3.068	3.051
Mn1-C8	3.014	2.976	3.199	3.159	3.068	3.061
Mn1-C9	2.230	2.212	3.582	3.518	2.331	2.300
Mn1-C10	2.175	2.147	3.190	3.178	2.177	2.156
Mn2-C4	2.198	2.195	2.240	2.202	2.269	2.246
Mn2-C5	2.179	2.165	2.180	2.149	2.187	2.172
Mn2-C6	2.162	2.144	2.258	2.187	2.145	2.118
Mn2-C7	2.179	2.165	2.286	2.220	2.216	2.159
Mn2-C8	2.198	2.195	2.273	2.243	2.261	2.218
C1-C2	1.425	1.432	1.441	1.449	1.431	1.436
C2-C3	1.426	1.439	1.402	1.415	1.406	1.425
C3-C4	1.482	1.479	1.465	1.468	1.476	1.477
C8-C9	1.482	1.479	1.456	1.456	1.479	1.483
C9-C10	1.426	1.439	1.353	1.367	1.407	1.422
C10-C1	1.425	1.432	1.477	1.476	1.429	1.437
C4-C8	1.414	1.430	1.458	1.468	1.420	1.428
C4-C5	1.436	1.445	1.452	1.459	1.419	1.430
C5-C6	1.431	1.441	1.420	1.432	1.449	1.455
C6-C7	1.431	1.441	1.422	1.432	1.430	1.443
C7-C8	1.436	1.445	1.425	1.437	1.427	1.441

Table S4. Manganese-carbon and carbon-carbon distances (in Å) for the $C_{10}H_8Mn_2(CO)_4$ structures

	4T-1		4S-2		4T-3		4S-4	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
Mn1-C1	2.298	2.413	2.196	2.204	2.194	2.199	2.331	2.625
Mn1-C2	2.109	2.125	2.160	2.160	2.157	2.153	2.096	2.136
Mn1-C3	2.123	2.153	2.122	2.127	2.128	2.114	2.101	1.103
Mn1-C4	2.582	2.724	2.380	2.328	2.389	2.366	2.559	2.642
Mn1-C8	3.262	3.305	2.390	2.344	2.407	2.342	3.307	3.309
Mn1-C9	3.605	3.550	2.118	2.112	2.121	2.125	3.658	3.633
Mn1-C10	3.208	3.167	2.153	2.150	2.157	2.154	3.249	3.333
Mn2-C4	2.179	2.136	2.201	2.187	2.280	2.213	2.190	2.104
Mn2-C5	2.150	2.120	2.173	2.152	2.213	2.152	2.123	2.107
Mn2-C6	2.203	2.181	2.151	2.110	2.191	2.150	2.144	2.141
Mn2-C7	2.280	2.230	2.156	2.106	2.186	2.177	2.187	2.158
Mn2-C8	2.246	2.199	2.203	2.186	2.235	2.248	2.241	2.202
C1-C2	1.429	1.430	1.426	1.431	1.428	1.433	1.433	1.432
C2-C3	1.409	1.426	1.415	1.427	1.412	1.424	1.409	1.432
C3-C4	1.465	1.459	1.460	1.452	1.459	1.457	1.467	1.461
C8-C9	1.456	1.454	1.461	1.454	1.462	1.452	1.448	1.433
C9-C10	1.357	1.380	1.409	1.423	1.412	1.426	1.362	1.393
C10-C1	1.465	1.448	1.429	1.433	1.427	1.433	1.453	1.426
C4-C8	1.471	1.472	1.462	1.482	1.461	1.482	1.474	1.484
C4-C5	1.440	1.448	1.434	1.449	1.431	1.453	1.442	1.452
C5-C6	1.428	1.444	1.430	1.435	1.428	1.433	1.425	1.434
C6-C7	1.426	1.430	1.418	1.435	1.420	1.436	1.434	1.438
C7-C8	1.420	1.439	1.446	1.455	1.445	1.444	1.420	1.448

Table S5. Manganese-carbon and carbon-carbon distances (in Å) for the singlet $C_{10}H_8Mn_2(CO)_3$ structures

	3S-1		3S-2		3T-3		3T-4	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
Mn1-C1	2.129	2.117	2.128	2.129	2.145	2.102	2.332	2.270
Mn1-C2	2.104	2.081	2.131	2.106	2.099	2.067	2.122	2.086
Mn1-C3	2.437	2.443	2.197	2.138	2.242	2.210	2.196	2.130
Mn1-C4	2.845	2.847	2.775	2.742	2.798	2.779	2.712	2.691
Mn1-C8	2.517	2.495	3.079	3.102	3.225	3.217	2.226	3.215
Mn1-C9	2.102	2.081	2.625	2.658	3.376	3.378	3.480	3.529
Mn1-C10	2.133	2.127	2.188	2.166	2.958	2.946	3.104	3.136
Mn2-C4	2.033	2.040	2.128	2.124	2.157	2.137	2.191	2.144
Mn2-C5	2.133	2.130	2.191	2.167	2.137	2.119	2.215	2.172
Mn2-C6	2.231	2.213	2.191	2.169	2.187	2.169	2.227	2.198
Mn2-C7	2.200	2.172	2.092	2.079	2.233	2.212	2.175	2.163
Mn2-C8	2.129	2.124	2.014	2.000	2.220	2.201	2.140	2.129
C1-C2	1.422	1.439	1.430	1.433	1.443	1.455	1.423	1.431
C2-C3	1.445	1.451	1.411	1.434	1.408	1.421	1.419	1.435
C3-C4	1.449	1.456	1.436	1.471	1.448	1.452	1.445	1.458
C8-C9	1.459	1.460	1.426	1.439	1.461	1.463	1.460	1.462
C9-C10	1.418	1.436	1.422	1.442	1.360	1.370	1.366	1.371
C10-C1	1.424	1.425	1.465	1.432	1.468	1.473	1.455	1.466
C4-C8	1.467	1.479	1.427	1.478	1.459	1.468	1.454	1.463
C4-C5	1.442	1.456	1.425	1.440	1.436	1.446	1.441	1.451
C5-C6	1.427	1.434	1.432	1.436	1.431	1.442	1.419	1.433
C6-C7	1.421	1.432	1.440	1.439	1.428	1.436	1.424	1.431
C7-C8	1.439	1.454	1.427	1.456	1.424	1.437	1.442	1.455

Table S6. Mangnanese-carbon and carbon-carbon distances (in Å) for the triplet $C_{10}H_8Mn_2(CO)_2$ structures

	2T-1		2S-2
	B3LYP	BP86	B3LYP
Mn1-C1	2.134	2.118	2.191
Mn1-C2	2.180	2.166	2.160
Mn1-C3	2.701	2.733	2.074
Mn1-C4	3.087	3.093	2.389
Mn1-C8	2.644	3.607	2.793
Mn1-C9	2.130	2.071	2.508
Mn1-C10	2.152	2.126	2.252
Mn2-C4	2.000	2.000	2.081
Mn2-C5	2.112	2.110	2.154
Mn2-C6	2.216	2.192	2.224
Mn2-C7	2.198	2.165	2.127
Mn2-C8	2.130	2.122	1.984
C1-C2	1.428	1.439	1.419
C2-C3	1.444	1.451	1.421
C3-C4	1.440	1.444	1.456
C8-C9	1.463	1.467	1.450
C9-C10	1.426	1.444	1.425
C10-C1	1.419	1.424	1.426
C4-C8	1.469	1.481	1.481
C4-C5	1.448	1.460	1.452
C5-C6	1.428	1.437	1.418
C6-C7	1.421	1.432	1.427
C7-C8	1.439	1.452	1.443

Table S7. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **6S-1** of $(C_{10}H_8)Mn_2(CO)_6$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	9(0)	11(0)	a	483(8)	491(3)	a	1048(9)	1018(7)
	44(0)	43(0)		492(3)	502(1)		1073(1)	1041(1)
	49(2)	49(1)		497(1)	512(2)		1172(1)	1133(1)
	50(1)	52(1)		527(47)	525(3)		1201(1)	1161(2)
	77(0)	75(0)		531(14)	533(21)		1218(2)	1174(1)
	81(0)	80(0)		537(14)	539(10)		1262(3)	1219(2)
	87(0)	86(0)		544(60)	546(34)		1277(8)	1238(6)
	88(0)	86(0)		584(8)	566(3)		1376(4)	1323(4)
	92(0)	90(0)		607(6)	588(4)		1403(3)	1360(2)
	107(1)	104(1)		607(49)	603(39)		1410(2)	1366(3)
	109(0)	107(0)		638(58)	629(49)		1454(0)	1401(0)
	121(0)	119(0)		645(130)	644(127)		1461(9)	1412(6)
	136(0)	135(1)		650(18)	646(25)		1503(6)	1470(2)
	152(2)	160(2)		665(0)	646(11)		1528(2)	1476(2)
	169(1)	170(1)		671(113)	666(77)		1561(1)	1505(0)
	186(0)	201(0)		682(92)	678(95)		1572(12)	1511(11)
	250(23)	260(33)		703(11)	688(19)		2018(776)	1936(658)
	327(1)	329(1)		774(0)	745(0)		2024(731)	1943(1)
	332(0)	330(1)		823(17)	794(13)		2031(951)	1944(1415)
	349(13)	357(5)		831(19)	808(16)		2037(967)	1959(816)
	362(7)	358(8)		871(4)	845(2)		2078(2295)	1998(1914)
	402(1)	397(2)		873(4)	847(7)		2092(166)	2012(159)
	408(0)	408(0)		884(9)	859(9)		3167(3)	3094(3)
	420(1)	415(0)		898(1)	865(0)		3167(0)	3094(0)
	428(3)	422(7)		913(6)	880(4)		3181(3)	3106(3)
	450(0)	439(1)		918(5)	883(1)		3181(9)	3107(8)
	468(4)	473(5)		976(2)	953(0)		3220(2)	3141(2)
	472(2)	476(0)		1004(0)	954(2)		3240(0)	3167(0)
	480(2)	482(9)		1017(2)	969(1)		3242(0)	3170(0)
	483(0)	484(0)		1029(2)	993(2)		3269(0)	3194(0)

Table S8. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **6S-2** of $(C_{10}H_8)Mn_2(CO)_6$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	25(0)	25(0)	a	487(9)	503(4)	a	1051(2)	1020(2)
	49(0)	48(0)		493(1)	507(1)		1076(1)	1042(1)
	50(0)	48(0)		501(2)	508(2)		1151(2)	1113(2)
	64(0)	65(0)		536(32)	535(3)		1195(2)	1151(1)
	85(0)	83(0)		540(55)	538(13)		1196(2)	1156(3)
	86(0)	83(0)		541(15)	543(35)		1240(5)	1196(4)
	88(0)	86(0)		548(8)	550(5)		1259(1)	1222(1)
	92(0)	91(0)		596(2)	575(4)		1356(3)	1303(4)
	97(1)	95(1)		615(49)	607(3)		1399(2)	1354(1)
	107(0)	105(0)		630(10)	613(43)		1417(1)	1369(1)
	112(0)	109(0)		644(89)	644(59)		1438(1)	1388(2)
	118(0)	117(0)		646(64)	644(102)		1445(6)	1394(7)
	145(0)	144(0)		651(42)	648(29)		1488(5)	1449(2)
	155(0)	156(0)		671(75)	651(2)		1526(0)	1470(0)
	194(1)	196(0)		678(0)	667(70)		1536(1)	1474(1)
	215(1)	232(1)		683(102)	680(73)		1555(39)	1500(34)
	231(4)	237(9)		708(10)	694(26)		2021(1196)	1942(976)
	334(4)	342(0)		767(0)	742(0)		2025(364)	1944(36)
	346(7)	344(9)		829(25)	805(21)		2034(1229)	1948(1308)
	347(0)	356(4)		846(1)	813(2)		2047(377)	1969(434)
	381(7)	380(8)		847(61)	818(49)		2078(858)	2000(662)
	386(11)	388(9)		874(8)	844(5)		2102(1136)	2022(905)
	409(0)	411(0)		885(6)	860(4)		3163(3)	3090(4)
	422(1)	421(0)		888(3)	862(8)		3164(0)	3091(1)
	457(8)	448(10)		924(0)	891(2)		3177(5)	3104(5)
	457(4)	454(0)		934(6)	898(3)		3177(11)	3104(9)
	468(1)	469(9)		977(2)	952(2)		3213(5)	3133(6)
	475(1)	479(0)		1003(0)	955(0)		3240(0)	3166(1)
	483(0)	488(1)		1024(1)	978(0)		3252(0)	3180(0)
	486(0)	489(0)		1030(2)	993(2)		3260(1)	3186(1)

Table S9 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **6T-3** of $(C_{10}H_8)Mn_2(CO)_6$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	9(0)	11(0)	a	449(34)	477(8)	a	1063(9)	1032(4)
	22(2)	28(0)		463(5)	480(4)		1082(5)	1045(1)
	29(2)	39(1)		479(1)	486(1)		1182(1)	1131(1)
	39(1)	43(2)		480(2)	504(2)		1213(6)	1155(1)
	43(1)	60(0)		489(0)	506(8)		1221(1)	1189(6)
	58(1)	74(0)		501(0)	532(20)		1260(1)	1217(1)
	66(1)	80(0)		520(39)	537(4)		1279(5)	1236(4)
	79(1)	83(0)		535(36)	539(32)		1376(1)	1322(2)
	86(0)	86(1)		541(35)	559(15)		1401(6)	1351(1)
	87(0)	94(1)		554(53)	571(4)		1421(3)	1375(2)
	89(1)	102(0)		586(19)	586(27)		1440(2)	1394(6)
	102(1)	103(0)		620(12)	616(14)		1452(4)	1401(1)
	107(1)	117(2)		634(50)	625(145)		1506(6)	1441(4)
	119(1)	134(5)		643(71)	632(35)		1511(9)	1457(3)
	150(1)	140(9)		662(24)	633(31)		1540(13)	1482(16)
	163(0)	148(4)		676(12)	660(34)		1631(92)	1503(5)
	270(9)	277(14)		681(80)	673(62)		1998(922)	1931(634)
	293(4)	292(8)		760(11)	719(14)		2026(678)	1940(492)
	313(9)	322(1)		782(18)	742(2)		2027(867)	1944(909)
	325(8)	342(6)		836(17)	805(3)		2033(1805)	1945(837)
	333(4)	363(3)		839(19)	813(14)		2074(2479)	1978(2406)
	337(14)	380(1)		861(2)	826(2)		2090(65)	2004(409)
	340(10)	387(5)		882(3)	834(6)		3166(3)	3099(2)
	345(1)	401(2)		890(1)	845(1)		3173(2)	3103(1)
	374(1)	403(9)		907(11)	869(1)		3183(3)	3115(1)
	396(19)	413(8)		916(2)	882(1)		3187(8)	3121(4)
	405(0)	428(10)		926(4)	897(0)		3198(6)	3133(1)
	422(7)	442(5)		973(0)	927(1)		3241(0)	3170(0)
	435(8)	457(4)		978(0)	937(1)		3244(0)	3175(0)
	446(16)	472(2)		1034(3)	1002(3)		3268(0)	3191(0)

Table S10. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **6T-4** of $(C_{10}H_8)Mn_2(CO)_6$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	28(0)	33(0)	a	448(21)	470(10)	a	1073(2)	1035(5)
	48(0)	44(0)		471(7)	474(1)		1086(9)	1058(2)
	54(0)	49(0)		472(32)	483(5)		1161(3)	1141(0)
	54(0)	60(0)		476(7)	487(3)		1218(7)	1192(3)
	62(0)	78(0)		478(37)	502(5)		1244(3)	1206(1)
	82(0)	80(0)		485(10)	505(6)		1249(5)	1222(0)
	84(2)	86(1)		499(13)	515(3)		1287(6)	1247(5)
	90(0)	90(0)		524(22)	549(8)		1377(4)	1337(6)
	93(0)	97(1)		572(4)	561(133)		1387(16)	1357(3)
	100(0)	99(0)		581(0)	582(13)		1432(11)	1379(2)
	106(0)	101(0)		603(23)	583(24)		1445(0)	1411(0)
	113(0)	112(1)		615(2)	593(44)		1446(10)	1414(1)
	119(1)	130(0)		630(38)	609(35)		1484(26)	1438(7)
	141(2)	140(0)		639(34)	613(15)		1514(36)	1479(26)
	151(3)	154(1)		658(14)	642(64)		1579(67)	1507(3)
	157(0)	195(4)		669(44)	648(22)		1665(29)	1576(9)
	167(1)	206(3)		671(157)	668(12)		2006(441)	1839(464)
	278(3)	212(3)		742(63)	703(49)		2012(320)	1876(173)
	295(2)	291(1)		758(24)	742(7)		2038(1017)	1939(819)
	313(2)	312(3)		820(11)	787(1)		2046(1621)	1944(397)
	335(1)	324(2)		836(43)	815(30)		2064(1389)	1965(1349)
	373(19)	332(3)		845(12)	824(1)		2108(888)	1999(1115)
	384(4)	372(5)		865(3)	832(9)		3148(1)	3090(2)
	401(9)	402(2)		879(8)	837(2)		3158(1)	3095(2)
	405(1)	406(20)		906(12)	871(6)		3162(7)	3108(6)
	409(10)	414(1)		920(8)	882(3)		3177(15)	3114(5)
	414(11)	426(0)		938(3)	917(1)		3190(26)	3122(10)
	423(1)	431(4)		991(1)	943(1)		3239(1)	3169(1)
	431(0)	440(2)		996(1)	954(0)		3248(0)	3175(0)
	439(3)	453(26)		1038(3)	1009(3)		3261(0)	3190(0)

Table S11. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5S-1** of $(C_{10}H_8)Mn_2(CO)_5$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	37(0)	35(0)	a	510(3)	506(0)	a	1082(3)	1051(1)
	44(0)	44(0)		515(21)	515(3)		1172(0)	1131(0)
	60(4)	61(6)		530(15)	534(6)		1222(3)	1191(4)
	67(0)	69(1)		531(31)	538(6)		1238(1)	1198(0)
	69(0)	70(0)		541(24)	543(12)		1266(12)	1225(12)
	98(1)	96(1)		548(1)	545(20)		1291(5)	1254(4)
	102(1)	101(0)		587(86)	581(12)		1381(3)	1331(2)
	105(0)	104(0)		609(24)	587(101)		1405(2)	1363(6)
	112(1)	112(0)		625(69)	620(22)		1425(0)	1378(0)
	119(0)	119(0)		629(37)	621(55)		1449(1)	1405(1)
	132(1)	136(1)		657(19)	637(12)		1465(2)	1413(1)
	144(1)	149(8)		667(63)	647(27)		1515(16)	1477(35)
	164(11)	163(12)		667(4)	659(38)		1515(50)	1499(3)
	217(3),	238(6)		677(39)	671(53)		1568(1)	1531(77)
	246(0)	256(0)		771(2)	745(2)		1584(69)	1531(2)
	314(8)	307(0)		826(0)	790(1)		1992(201)	1908(145)
	325(0)	323(14)		826(18)	797(10)		2022(99)	1939(153)
	340(3)	330(2)		840(62)	812(66)		2037(1223)	1953(1009)
	341(9)	350(3)		861(14)	833(17)		2038(1586)	1958(1203)
	388(14)	386(11)		863(4)	834(2)		2090(1256)	2008(1022)
	402(1)	395(2)		882(9)	861(4)		3172(1)	3099(1)
	421(1)	405(1)		902(3)	869(0)		3172(0)	3100(0)
	427(7)	420(6)		940(7)	899(7)		3186(1)	3110(1)
	459(2)	456(0)		955(5)	926(0)		3188(7)	3113(6)
	468(0)	472(5)		980(0)	930(8)		3210(6)	3127(8)
	472(1)	475(1)		986(10)	941(1)		3245(0)	3172(0)
	475(1)	483(0)		1036(3)	1005(4)		3253(0)	3179(0)
	489(0)	497(3)		1060(1)	1031(1)		3265(0)	3191(0)

Table S12. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5S-2** of $(C_{10}H_8)Mn_2(CO)_5$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	39(1)	40(1)	a	505(5)	505(7)	a	1072(3)	1040(1)
	46(0)	51(0)		526(5)	528(3)		1164(1)	1125(1)
	65(0)	65(0)		532(28)	534(5)		1201(1)	1160(1)
	72(0)	69(0)		538(15)	539(6)		1224(4)	1184(4)
	85(0)	85(0)		549(65)	562(47)		1252(5)	1212(3)
	95(1)	92(0)		587(56)	568(12)		1279(2)	1233(2)
	100(0)	97(0)		595(72)	582(11)		1370(3)	1321(2)
	109(1)	106(0)		604(76)	594(155)		1391(1)	1351(2)
	110(0)	107(0)		621(15)	609(15)		1419(0)	1366(0)
	120(0)	119(0)		632(53)	627(50)		1434(2)	1393(2)
	125(0)	129(0)		656(22)	648(18)		1455(5)	1403(5)
	168(1)	170(1)		665(112)	657(93)		1491(10)	1451(1)
	186(16)	190(17)		691(1)	674(3)		1518(7)	1473(3)
	242(3)	252(2)		754(8)	732(8)		1528(5)	1483(3)
	279(6)	285(8)		798(12)	780(8)		1572(8)	1527(5)
	307(4)	308(1)		831(16)	803(15)		2007(120)	1925(224)
	320(5)	330(9)		835(13)	805(12)		2012(5)	1935(79)
	343(25)	348(12)		850(9)	826(11)		2031(1213)	1949(968)
	386(10)	386(9)		861(5)	831(5)		2034(1862)	1960(1299)
	397(2)	395(3)		880(4)	842(4)		2087(1360)	2006(1067)
	420(2)	413(1)		897(9)	858(9)		3171(2)	3097(2)
	423(1)	418(4)		911(8)	870(5)		3173(2)	3098(2)
	443(14)	441(7)		917(2)	884(3)		3190(2)	3112(2)
	455(10)	456(4)		937(1)	906(0)		3197(4)	3118(5)
	468(1)	466(4)		970(2)	933(2)		3208(4)	3130(5)
	476(1)	478(2)		990(1)	953(1)		3239(0)	3166(0)
	479(1)	483(1)		1031(3)	999(3)		3247(0)	3173(0)
	488(1)	495(1)		1062(7)	1033(7)		3264(0)	3190(1)

Table S13. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5S-3** of $(C_{10}H_8)Mn_2(CO)_5$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	22(0)	2(0)	a	492(2)	502(2)	a	1070(3)	1037(2)
	40(1)	41(1)		495(10)	507(4)		1168(1)	1135(1)
	43(0)	41(0)		526(46)	524(2)		1199(2)	1163(3)
	47(1)	47(1)		531(7)	535(15)		1214(5)	1175(2)
	71(0)	72(0)		556(38)	555(8)		1258(3)	1224(2)
	81(1)	80(0)		571(45)	566(28)		1272(1)	1238(1)
	87(0)	86(0)		584(25)	574(48)		1372(4)	1325(4)
	95(1)	94(1)		607(59)	604(57)		1389(1)	1354(2)
	104(0)	103(0)		617(12)	605(53)		1413(5)	1368(1)
	111(0)	109(0)		647(52)	642(52)		1446(9)	1398(2)
	129(2)	130(1)		653(71)	648(19)		1460(16)	1408(19)
	145(1)	144(1)		671(100)	651(57)		1497(6)	1467(1)
	164(3)	162(2)		680(6)	665(68)		1526(3)	1469(5)
	178(1)	168(1)		696(12)	676(47)		1553(24)	1501(2)
	239(13)	226(32)		770(1)	739(0)		1571(3)	1512(3)
	328(0)	328(16)		827(13)	804(3)		1992(1033)	1906(811)
	344(6)	334(0)		832(34)	811(30)		2030(814)	1944(671)
	356(4)	350(0)		862(5)	836(7)		2037(1475)	1946(2025)
	363(9)	371(6)		870(1)	840(2)		2042(1469)	1959(704)
	402(0)	404(1)		878(3)	852(7)		2090(899)	2009(884)
	403(1)	408(1)		883(10)	854(8)		3165(2)	3095(2)
	419(2)	414(0)		909(5)	868(3)		3166(2)	3095(2)
	435(6)	433(1)		915(3)	880(1)		3179(5)	3107(3)
	449(0)	436(12)		971(2)	947(1)		3180(9)	3108(7)
	468(5)	472(5)		1000(0)	951(1)		3216(3)	3138(2)
	472(3)	477(1)		1014(3)	966(1)		3238(0)	3165(0)
	483(8)	481(0)		1026(3)	992(1)		3244(0)	3169(0)
	485(1)	494(2)		1042(12)	1013(10)		3265(0)	3190(0)

Table S14. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5T-4** of $(C_{10}H_8)Mn_2(CO)_5$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	9(0)	10(0)	a	487(19)	495(8)	a	1069(0)	1038(0)
	29(0)	29(0)		492(4)	507(1)		1146(5)	1113(3)
	35(1)	30(1)		494(1)	522(22)		1182(7)	1147(1)
	61(0)	60(0)		537(16)	540(15)		1194(1)	1159(2)
	77(0)	75(0)		541(31)	547(0)		1237(11)	1202(8)
	81(1)	79(1)		548(11)	550(21)		1260(1)	1222(1)
	88(0)	86(0)		581(5)	555(4)		1352(7)	1303(5)
	90(0)	88(0)		589(24)	588(1)		1395(3)	1351(1)
	104(0)	103(0)		620(3)	601(18)		1414(4)	1366(1)
	105(0)	105(0)		643(81)	640(85)		1429(0)	1381(2)
	134(3)	131(4)		645(52)	640(45)		1446(4)	1398(2)
	150(0)	150(0)		679(0)	651(0)		1483(21)	1452(5)
	205(1)	202(1)		683(87)	675(61)		1516(16)	1458(1)
	235(1)	240(2)		705(7)	688(15)		1519(0)	1473(1)
	240(1)	245(2)		763(3)	741(1)		1542(41)	1482(9)
	305(4)	320(3)		819(31)	781(26)		2011(6)	1924(238)
	338(15)	333(0)		842(47)	811(36)		2020(745)	1941(391)
	341(0)	346(2)		848(1)	815(2)		2028(1837)	1946(1150)
	349(1)	346(15)		859(17)	834(4)		2065(1041)	1966(1416)
	369(15)	364(7)		871(0)	835(3)		2089(1213)	2006(871)
	375(1)	377(7)		883(0)	853(2)		3156(4)	3088(2)
	407(8)	407(0)		924(3)	886(8)		3157(0)	3089(0)
	407(23)	423(6)		932(3)	896(0)		3169(5)	3098(2)
	438(24)	435(1)		962(1)	901(0)		3170(9)	3100(8)
	449(1)	449(0)		973(8)	935(2)		3202(8)	3120(9)
	453(12)	476(34)		998(0)	956(2)		3239(0)	3167(0)
	477(4)	478(2)		1019(4)	986(3)		3252(0)	3180(0)
	485(1)	485(7)		1049(2)	1019(1)		3259(2)	3186(1)

Table S15. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5T-5** of $(C_{10}H_8)Mn_2(CO)_5$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	37(0)	38(0)	a	476(22)	491(3)	a	1090(2)	1059(1)
	47(0)	39(0)		479(17)	498(2)		1168(3)	1134(0)
	61(0)	58(0)		491(0)	504(27)		1193(4)	1155(2)
	63(0)	66(0)		510(15)	510(13)		1208(4)	1173(4)
	73(0)	76(0)		519(16)	515(49)		1241(3)	1205(2)
	87(1)	87(1)		529(20)	533(24)		1262(2)	1222(2)
	93(0)	94(0)		566(5)	536(10)		1368(2)	1320(2)
	101(0)	97(0)		596(21)	569(18)		1387(8)	1345(2)
	106(0)	106(0)		606(13)	593(21)		1424(17)	1380(2)
	108(0)	117(0)		615(51)	597(22)		1433(3)	1385(6)
	126(0)	126(0)		627(33)	614(29)		1442(3)	1393(5)
	140(0)	153(2)		659(71)	627(18)		1464(8)	1425(4)
	156(3)	162(0)		662(7)	633(58)		1512(19)	1467(16)
	197(1)	194(5)		680(14)	658(8)		1534(25)	1487(11)
	269(1)	261(0)		758(21)	724(24)		1664(12)	1590(4)
	281(1)	287(4)		780(9)	751(7)		1992(106)	1903(196)
	306(4)	318(5)		829(21)	801(15)		2010(277)	1922(9)
	330(6)	343(1)		831(38)	806(26)		2023(1547)	1941(1040)
	349(4)	348(3)		853(6)	823(3)		2048(1498)	1955(1735)
	382(14)	373(14)		875(8)	845(11)		2091(1311)	1999(1028)
	386(4)	384(2)		882(4)	849(3)		3153(4)	3081(3)
	395(1)	388(3)		895(1)	872(1)		3166(11)	3095(9)
	418(14)	414(4)		921(4)	881(8)		3180(7)	3107(6)
	427(2)	448(1)		943(2)	897(0)		3192(13)	3118(10)
	448(20)	449(5)		967(2)	915(3)		3202(7)	3124(6)
	459(5)	456(0)		992(1)	944(1)		3235(0)	3163(0)
	468(5)	466(3)		1041(1)	1007(2)		3240(0)	3168(0)
	469(6)	474(5)		1073(9)	1041(8)		3261(0)	3188(0)

Table S16. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **5T-6** of $(C_{10}H_8)Mn_2(CO)_5$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	18(0)	16(0)	a	477(13)	487(1)	a	1070(2)	1037(1)
	45(1)	43(1)		483(8)	499(27)		1167(1)	1126(1)
	47(1)	45(1)		491(5)	502(1)		1194(3)	1155(3)
	49(1)	51(1)		523(73)	525(2)		1212(2)	1167(1)
	70(0)	68(0)		528(78)	533(20)		1255(3)	1211(2)
	82(0)	80(0)		533(5)	547(57)		1268(3)	1228(1)
	84(0)	83(0)		578(6)	556(16)		1370(4)	1316(4)
	90(0)	89(0)		601(13)	588(1)		1383(0)	1340(1)
	100(1)	98(0)		607(57)	603(54)		1402(4)	1356(3)
	105(0)	105(0)		613(44)	618(37)		1448(1)	1392(2)
	123(1)	126(0)		648(58)	646(35)		1458(16)	1408(13)
	148(1)	151(1)		670(2)	646(19)		1498(6)	1462(2)
	170(1)	172(2)		671(108)	665(91)		1533(3)	1480(2)
	187(1)	205(1)		702(6)	686(19)		1553(8)	1493(1)
	246(10)	255(15)		773(1)	744(1)		1568(6)	1504(21)
	304(5)	312(1)		810(28)	777(16)		1976(1695)	1895(1188)
	312(2)	325(4)		830(19)	805(8)		2028(800)	1943(664)
	338(4)	347(3)		842(3)	808(14)		2036(942)	1957(1185)
	356(2)	354(3)		867(2)	829(2)		2059(542)	1961(898)
	376(4)	375(3)		876(10)	846(12)		2089(821)	2009(859)
	396(2)	395(1)		878(8)	853(4)		3164(2)	3092(2)
	418(4)	412(0)		890(1)	862(4)		3166(1)	3094(1)
	419(13)	425(4)		916(5)	886(1)		3178(7)	3104(6)
	427(16)	438(4)		975(2)	951(3)		3180(8)	3106(7)
	451(0)	442(1)		1003(0)	952(1)		3216(3)	3136(3)
	466(2)	473(7)		1018(2)	970(1)		3235(0)	3163(0)
	470(4)	476(1)		1025(4)	990(2)		3242(0)	3171(0)
	473(2)	481(1)		1036(8)	1006(9)		3260(0)	3185(0)

Table S17. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4T-1** of $(C_{10}H_8)Mn_2(CO)_4$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	37(1)	29(1)	a	495(57)	505(9)	a	1177(1)	1138(0)
	59(0)	55(0)		511(26)	517(11)		1200(8)	1175(1)
	64(0)	67(0)		516(4)	525(23)		1208(6)	1187(3)
	82(1)	75(1)		519(7)	529(5)		1250(8)	1215(7)
	94(0)	90(0)		563(29)	549(35)		1268(3)	1239(1)
	101(1)	92(1)		574(17)	565(32)		1371(6)	1328(1)
	111(0)	107(1)		583(34)	583(15)		1376(15)	1353(2)
	143(2)	129(0)		622(9)	619(45)		1423(6)	1373(1)
	147(2)	137(1)		635(46)	631(9)		1432(5)	1396(3)
	173(8)	143(2)		664(10)	644(17)		1451(6)	1406(4)
	196(5)	164(6)		677(2)	653(5)		1477(38)	1445(2)
	209(2)	203(1)		748(28)	723(26)		1511(31)	1470(5)
	215(2)	265(1)		775(10)	745(2)		1544(12)	1509(4)
	283(2)	277(6)		818(9)	781(23)		1649(21)	1551(5)
	303(2)	303(6)		829(26)	801(14)		1852(399)	1696(231)
	342(0)	357(3)		842(17)	812(4)		1989(352)	1903(215)
	363(18)	372(2)		853(8)	824(3)		2029(2367)	1937(1616)
	380(70)	385(8)		882(8)	852(2)		2067(1474)	1971(1313)
	385(1)	407(2)		899(3)	863(0)		3153(5)	3091(2)
	394(4)	412(5)		909(3)	872(7)		3167(13)	3102(2)
	417(6)	431(9)		920(3)	889(4)		3179(4)	3107(2)
	443(2)	442(7)		959(15)	914(2)		3190(15)	3114(12)
	458(6)	455(4)		974(4)	923(1)		3194(9)	3122(6)
	458(12)	469(3)		1038(3)	1005(5)		3234(1)	3160(0)
	483(31)	487(7)		1063(11)	1030(12)		3239(1)	3173(0)
	493(50)	497(2)		1086(3)	1056(0)		3259(1)	3189(1)

Table S18. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4S-2** of $(C_{10}H_8)Mn_2(CO)_4$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	27(0)	32(1)	a	522(21)	522(4)	a	1171(2)	1130(2)
	43(1)	44(1)		528(33)	539(10)		1199(6)	1164(2)
	55(2)	52(1)		548(7)	545(17)		1215(6)	1189(6)
	60(0)	58(1)		553(4)	553(12)		1237(1)	1202(1)
	77(0)	77(0)		565(65)	572(42)		1270(5)	1234(2)
	95(1)	96(1)		574(43)	577(36)		1360(7)	1314(5)
	100(0)	100(0)		612(6)	591(16)		1368(8)	1323(6)
	104(0)	105(0)		647(52)	619(8)		1427(0)	1380(0)
	139(1)	140(3)		651(46)	643(18)		1434(0)	1385(1)
	145(0)	154(4)		663(1)	647(69)		1456(0)	1411(1)
	162(1)	160(0)		685(0)	672(2)		1474(3)	1437(1)
	282(2)	281(5)		779(2)	751(2)		1492(19)	1474(4)
	290(3)	291(4)		802(1)	764(5)		1536(9)	1493(7)
	321(1)	320(0)		809(21)	784(18)		1544(3)	1505(6)
	333(4)	328(4)		833(9)	808(4)		1995(716)	1906(494)
	337(7)	344(1)		842(12)	815(4)		2002(1147)	1912(864)
	353(0)	362(9)		854(11)	821(15)		2039(3020)	1951(2511)
	396(1)	396(1)		876(11)	846(7)		2057(133)	1970(291)
	402(1)	404(5)		913(0)	876(0)		3175(1)	3098(1)
	421(8)	414(6)		927(1)	887(2)		3186(2)	3110(2)
	452(1)	434(4)		937(5)	893(3)		3193(4)	3116(3)
	456(1)	451(7)		945(4)	915(3)		3203(5)	3123(6)
	475(4)	481(2)		972(5)	927(5)		3205(4)	3126(4)
	482(3)	485(0)		1036(3)	1006(3)		3243(0)	3168(0)
	492(5)	496(2)		1063(5)	1032(6)		3251(0)	3174(0)
	508(1)	509(1)		1082(3)	1049(2)		3263(0)	3186(0)

Table S19. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4T-3** of $(C_{10}H_8)Mn_2(CO)_4$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	18(0)	22(0)	a	506(20)	504(12)	a	1172(2)	1132(1)
	42(1)	42(1)		522(54)	524(1)		1199(4)	1163(1)
	49(2)	48(2)		522(29)	536(17)		1213(5)	1185(6)
	59(0)	55(0)		530(16)	542(15)		1234(2)	1201(1)
	70(0)	71(0)		554(15)	551(64)		1270(5)	1233(2)
	85(0)	85(1)		556(27)	554(7)		1359(6)	1312(4)
	96(0)	96(0)		600(41)	583(0)		1368(5)	1322(3)
	99(1)	100(0)		610(18)	608(33)		1424(4)	1377(0)
	135(0)	137(2)		651(25)	612(13)		1435(2)	1387(1)
	145(0)	151(0)		652(9)	643(32)		1452(4)	1406(1)
	154(0)	155(3)		684(1)	670(3)		1478(3)	1438(2)
	273(1)	275(1)		780(2)	753(2)		1493(13)	1472(3)
	289(5)	291(4)		803(4)	780(1)		1538(1)	1493(4)
	305(6)	309(3)		812(32)	785(26)		1544(4)	1505(1)
	310(6)	323(1)		830(4)	800(7)		1988(1475)	1905(361)
	333(1)	326(5)		846(5)	812(3)		1991(925)	1905(1377)
	343(3)	338(4)		854(3)	817(2)		2039(2369)	1955(2773)
	358(1)	360(0)		875(10)	844(5)		2072(579)	1973(19)
	390(0)	385(1)		893(2)	850(2)		3176(1)	3099(1)
	410(15)	408(6)		916(1)	881(1)		3186(2)	3111(1)
	421(25)	433(3)		938(5)	892(3)		3193(4)	3115(4)
	444(3)	435(4)		944(3)	916(3)		3202(6)	3124(7)
	455(0)	441(0)		971(5)	927(4)		3204(4)	3125(4)
	462(0)	474(8)		1034(2)	1003(3)		3239(0)	3165(0)
	471(11)	480(3)		1063(12)	1033(10)		3247(0)	3174(0)
	476(5)	485(9)		1080(1)	1047(0)		3259(0)	3185(0)

Table S20. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4S-4** of $(C_{10}H_8)Mn_2(CO)_4$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	55(0)	47(0)	a	513(8)	514(2)	a	1180(3)	1134(2)
	67(0)	66(0)		520(49)	526(17)		1200(3)	1178(3)
	71(0)	74(1)		534(12)	543(11)		1210(2)	1196(2)
	88(1)	83(0)		554(15)	549(8)		1247(5)	1208(5)
	99(0)	87(1)		570(27)	559(1)		1269(7)	1243(2)
	102(0)	99(0)		586(30)	582(30)		1372(2)	1326(4)
	107(1)	103(0)		603(18)	584(21)		1379(2)	1343(2)
	138(0)	116(0)		633(13)	615(7)		1417(8)	1380(2)
	163(4)	127(4)		645(30)	631(10)		1435(2)	1394(2)
	169(0)	163(1)		664(4)	643(28)		1455(13)	1414(2)
	200(2)	178(3)		684(3)	655(10)		1471(40)	1439(15)
	213(0)	204(1)		751(26)	728(28)		1519(47)	1493(4)
	219(0)	243(2)		777(6)	740(9)		1538(10)	1505(1)
	305(2)	302(2)		820(15)	786(39)		1638(44)	1540(6)
	333(2)	328(5)		830(19)	805(5)		1865(415)	1696(280)
	347(2)	354(8)		850(9)	819(3)		1990(370)	1904(172)
	372(6)	377(5)		874(7)	828(5)		2032(1302)	1941(1241)
	382(9)	387(2)		881(3)	854(3)		2066(1473)	1974(1260)
	403(0)	408(3)		906(5)	866(4)		3151(5)	3088(3)
	418(8)	440(5)		917(6)	878(6)		3166(10)	3099(3)
	445(3)	444(6)		921(6)	897(2)		3177(7)	3104(2)
	460(6)	448(1)		960(7)	922(1)		3188(16)	3111(14)
	461(2)	460(1)		976(5)	936(1)		3193(8)	3118(8)
	481(19)	466(5)		1034(2)	1006(4)		3221(0)	3160(1)
	489(5)	484(3)		1063(13)	1031(12)		3238(1)	3169(0)
	508(36)	507(9)		1086(2)	1054(2)		3259(0)	3182(1)

Table S21 . Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3S-1** of $(C_{10}H_8)Mn_2(CO)_3$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	50(0)	46(0)	a	557(17)	545(8)	a	1195(3)	1153(2)
	60(1)	61(1)		561(39)	567(24)		1211(5)	1174(5)
	70(0)	71(0)		571(8)	576(75)		1241(2)	1197(1)
	92(1)	91(0)		598(81)	581(13)		1267(5)	1225(4)
	98(0)	98(1)		608(12)	595(26)		1359(3)	1309(3)
	110(1)	115(1)		657(39)	642(35)		1384(1)	1340(1)
	149(1)	141(1)		686(3)	667(2)		1416(1)	1363(0)
	173(2)	174(5)		744(1)	721(1)		1429(3)	1387(2)
	205(4)	212(4)		785(8)	760(9)		1444(1)	1393(2)
	269(1)	271(0)		808(22)	781(9)		1477(4)	1430(2)
	285(3)	284(5)		818(21)	783(16)		1502(5)	1454(2)
	298(10)	295(11)		840(11)	805(15)		1515(2)	1476(0)
	330(0)	337(1)		850(3)	818(3)		1540(5)	1496(0)
	350(6)	357(5)		857(14)	828(16)		1967(356)	1883(245)
	368(5)	372(7)		867(3)	836(5)		2005(1663)	1909(1254)
	411(0)	403(1)		898(4)	854(2)		2039(1366)	1952(1103)
	427(2)	407(2)		908(1)	864(5)		3168(1)	3088(1)
	429(4)	419(2)		927(2)	882(2)		3174(1)	3096(1)
	458(1)	454(2)		954(3)	917(1)		3185(4)	3104(4)
	463(4)	458(1)		968(1)	926(4)		3198(6)	3114(6)
	493(2)	487(3)		1025(5)	993(4)		3202(5)	3118(10)
	518(10)	517(3)		1065(5)	1035(6)		3241(0)	3168(0)
	530(21)	531(6)		1071(6)	1039(2)		3249(0)	3174(0)
	542(26)	539(10)		1163(3)	1122(2)		3266(0)	3192(0)

Table S22. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3S-2** of $(C_{10}H_8)Mn_2(CO)_3$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	28(2)	49(1)	a	558(60)	554(53)	a	1202(3)	1156(1)
	60(1)	64(1)		560(73)	558(24)		1216(4)	1177(4)
	81(1)	82(0)		571(37)	562(5)		1252(6)	1207(3)
	93(0)	94(0)		582(18)	581(52)		1274(4)	1230(4)
	111(5)	114(4)		608(2)	598(8)		1368(1)	1316(2)
	143(1)	146(1)		643(95)	652(64)		1392(1)	1348(0)
	176(0)	184(0)		686(3)	669(7)		1415(2)	1365(1)
	191(4)	193(6)		734(8)	723(5)		1427(1)	1380(2)
	234(4)	238(2)		778(8)	758(7)		1451(1)	1399(2)
	255(1)	262(1)		808(12)	778(5)		1492(8)	1444(0)
	293(4)	295(6)		818(23)	783(21)		1513(1)	1476(1)
	297(6)	307(11)		851(7)	819(6)		1531(4)	1484(1)
	325(8)	340(6)		856(11)	824(3)		1554(3)	1501(1)
	348(1)	360(4)		861(9)	832(14)		1798(341)	1709(261)
	375(8)	379(4)		874(1)	843(3)		2004(2035)	1915(1670)
	406(5)	402(3)		899(7)	858(5)		2028(1044)	1933(771)
	422(1)	415(1)		908(0)	875(0)		3157(2)	3080(1)
	447(5)	440(4)		931(1)	883(1)		3173(1)	3095(3)
	459(13)	456(4)		960(3)	919(1)		3190(4)	3110(2)
	476(3)	480(4)		972(2)	932(5)		3195(4)	3113(5)
	481(1)	481(4)		1030(3)	996(3)		3204(7)	3122(9)
	500(3)	494(2)		1060(12)	1031(8)		3234(0)	3160(0)
	526(6)	529(27)		1072(2)	1038(2)		3246(0)	3169(1)
	531(38)	535(15)		1169(1)	1127(1)		3264(0)	3190(0)

Table S23. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3T-3** of $(C_{10}H_8)Mn_2(CO)_3$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	48(0)	47(0)	a	541(18)	543(0)	a	1203(0)	1161(0)
	61(0)	59(0)		553(7)	549(16)		1217(2)	1182(1)
	83(1)	82(1)		572(58)	565(69)		1255(2)	1216(3)
	88(1)	88(0)		589(23)	586(4)		1277(1)	1234(1)
	108(1)	108(0)		607(11)	593(21)		1376(1)	1324(1)
	121(3)	117(2)		650(10)	637(4)		1398(5)	1360(1)
	143(5)	143(3)		665(2)	644(9)		1413(3)	1368(2)
	157(4)	156(5)		677(5)	660(3)		1433(3)	1385(1)
	191(1)	191(2)		760(21)	730(22)		1444(1)	1396(3)
	236(2)	274(2)		775(8)	749(8)		1460(2)	1425(2)
	271(3)	287(1)		816(30)	783(29)		1510(1)	1462(3)
	294(4)	313(3)		828(13)	796(13)		1558(10)	1518(3)
	312(6)	316(4)		855(2)	821(1)		1635(0)	1595(2)
	353(4)	352(4)		862(2)	825(2)		1700(344)	1624(239)
	361(3)	381(1)		873(14)	838(10)		2001(1516)	1915(1238)
	392(1)	401(1)		883(6)	847(5)		2022(1386)	1939(1034)
	425(8)	421(3)		892(5)	866(3)		3160(2)	3081(2)
	431(1)	428(0)		916(1)	878(2)		3164(1)	3084(1)
	450(7)	454(12)		947(1)	915(1)		3172(5)	3092(7)
	467(6)	456(4)		971(2)	928(3)		3188(15)	3111(14)
	471(0)	464(1)		1036(4)	1003(4)		3200(4)	3120(5)
	500(16)	504(6)		1060(12)	1029(11)		3236(0)	3162(0)
	504(28)	515(4)		1083(1)	1054(1)		3244(0)	3171(0)
	517(7)	529(10)		1179(0)	1139(0)		3264(0)	3190(0)

Table S24. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3T-4** of $(C_{10}H_8)Mn_2(CO)_3$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	43(1)	32(1)	a	508(5)	531(29)	a	1213(2)	1168(2)
	52(1)	65(0)		528(13)	540(22)		1217(3)	1182(1)
	78(1)	83(0)		546(3)	549(1)		1241(1)	1202(1)
	93(0)	97(1)		556(4)	558(14)		1273(1)	1228(1)
	104(3)	119(1)		596(41)	593(3)		1369(2)	1318(1)
	124(1)	132(1)		605(10)	627(12)		1396(7)	1355(2)
	151(2)	147(0)		660(12)	633(35)		1426(1)	1377(1)
	154(2)	157(1)		667(2)	657(1)		1437(3)	1388(3)
	177(5)	199(4)		745(25)	713(25)		1447(6)	1399(3)
	192(1)	205(2)		766(5)	743(4)		1454(0)	1451(3)
	218(2)	222(1)		807(22)	778(32)		1504(2)	1460(8)
	286(5)	289(6)		818(26)	789(8)		1540(5)	1494(4)
	292(5)	303(3)		837(4)	800(5)		1612(6)	1586(2)
	314(8)	354(1)		849(4)	818(0)		1771(558)	1717(423)
	360(0)	367(7)		856(3)	843(5)		1982(1656)	1888(837)
	371(6)	381(5)		890(4)	852(4)		2003(1181)	1922(1136)
	387(2)	400(12)		903(1)	868(2)		3161(2)	3073(2)
	400(34)	414(5)		909(3)	886(4)		3172(4)	3090(9)
	412(8)	430(9)		939(0)	912(1)		3181(1)	3100(2)
	436(1)	447(3)		966(2)	926(2)		3190(12)	3114(11)
	445(12)	460(7)		1035(4)	1001(4)		3200(5)	3116(7)
	470(1)	477(6)		1068(14)	1037(15)		3233(0)	3157(0)
	485(20)	494(1)		1081(3)	1050(1)		3243(0)	3166(0)
	489(53)	514(5)		1167(0)	1127(0)		3255(0)	3179(0)

Table S25. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **2T-1** of $(C_{10}H_8)Mn_2(CO)_2$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	62(1)	62(1)	a	605(24)	591(28)	a	1209(6)	1171(7)
	87(0)	83(0)		614(52)	602(47)		1234(5)	1190(3)
	115(1)	117(1)		675(13)	655(5)		1259(3)	1216(3)
	124(1)	122(2)		682(52)	661(43)		1355(2)	1306(3)
	189(3)	177(2)		740(9)	716(6)		1381(2)	1336(1)
	208(1)	206(3)		788(14)	767(12)		1409(0)	1356(0)
	223(7)	226(7)		802(16)	772(9)		1423(3)	1379(2)
	246(2)	256(1)		816(9)	782(7)		1446(1)	1395(2)
	285(5)	289(6)		827(40)	791(40)		1479(3)	1433(0)
	293(9)	297(11)		846(2)	809(2)		1494(1)	1459(1)
	342(2)	338(2)		846(3)	811(1)		1508(1)	1472(2)
	353(2)	366(5)		862(3)	829(2)		1521(5)	1480(1)
	378(4)	372(4)		891(3)	853(2)		1720(540)	1625(367)
	420(4)	410(2)		899(2)	857(2)		2015(1365)	1931(1124)
	432(1)	424(0)		906(1)	862(0)		3147(4)	3059(9)
	448(2)	440(2)		943(3)	905(0)		3150(4)	3063(4)
	477(3)	464(5)		953(4)	920(7)		3166(8)	3082(10)
	497(5)	484(7)		1025(6)	992(6)		3185(9)	3101(7)
	499(9)	496(1)		1062(7)	1032(5)		3187(8)	3107(9)
	527(5)	509(10)		1069(7)	1036(6)		3238(0)	3165(1)
	563(4)	538(1)		1157(2)	1116(2)		3249(1)	3175(1)
	572(48)	563(29)		1183(2)	1141(1)		3263(1)	3190(1)

Table S26. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **2S-2** of $(C_{10}H_8)Mn_2(CO)_2$

	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
a	38(1)	59(0)	a	566(0)	545(18)	a	1217(9)	1174(6)
	60(0)	67(0)		569(11)	580(3)		1230(4)	1187(2)
	83(1)	74(0)		613(5)	599(6)		1269(5)	1224(4)
	90(1)	88(1)		677(2)	689(4)		1352(6)	1308(3)
	131(3)	133(1)		739(4)	724(4)		1371(7)	1334(1)
	149(1)	160(1)		771(16)	753(3)		1419(0)	1358(0)
	221(3)	225(3)		788(14)	755(44)		1428(1)	1393(3)
	227(1)	256(2)		811(35)	772(18)		1447(4)	1394(1)
	289(3)	280(7)		818(4)	792(4)		1473(6)	1424(1)
	297(5)	310(1)		830(8)	797(3)		1498(5)	1445(7)
	311(3)	321(1)		849(2)	816(1)		1521(5)	1475(0)
	349(3)	357(1)		876(4)	843(1)		1529(3)	1487(3)
	374(3)	372(1)		891(0)	847(1)		1958(1027)	1886(795)
	416(2)	389(4)		906(3)	860(2)		2019(1566)	1936(1138)
	434(2)	429(2)		915(5)	889(1)		3167(2)	3079(7)
	446(4)	438(7)		942(9)	911(3)		3169(4)	3084(4)
	449(7)	472(3)		953(1)	927(8)		3182(3)	3106(1)
	500(6)	487(3)		1031(4)	988(6)		3197(6)	3109(9)
	507(8)	496(21)		1063(12)	1038(7)		3200(5)	3121(6)
	521(17)	506(20)		1077(3)	1041(7)		3235(0)	3161(0)
	545(57)	516(11)		1157(2)	1115(1)		3248(0)	3170(0)
	551(13)	538(1)		1191(1)	1147(0)		3262(0)	3187(0)

Table S27. Optimized coordinates for the $C_{10}H_8Mn_2(CO)_n$ (n = 6, 5, 4, 3, 2, 1) structures

6S-1

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.316481	-1.929796	0.000000	1.293553	-1.935714	0.000000
6	-1.110462	-1.290509	1.260951	1.115617	-1.283042	-1.265526
6	-0.601194	-0.000458	1.487822	0.620662	0.032249	-1.478861
6	-1.110461	-1.290487	-1.260963	1.115613	-1.282991	1.265585
6	0.449638	0.688385	0.714433	-0.452310	0.707068	-0.718953
6	-0.601206	-0.000424	-1.487808	0.620649	0.032304	1.478866
6	0.449630	0.688407	-0.714412	-0.452313	0.707093	0.718920
1	-1.746904	-2.927710	0.000000	1.723602	-2.943549	0.000000
1	-1.549583	-1.805539	2.115331	1.548398	-1.805861	-2.129007
1	-0.743161	0.376059	2.500870	0.787443	0.425098	-2.491172
1	-1.549573	-1.805507	-2.115355	1.548401	-1.805767	2.129089
1	-0.743173	0.376108	-2.500851	0.787426	0.425199	2.491160
6	1.438664	1.606059	1.155729	-1.464120	1.616173	-1.163998
1	1.667888	1.843481	2.189489	-1.701656	1.850295	-2.205284
6	2.074204	2.173420	0.000000	-2.105055	2.183114	0.000000
1	2.850721	2.928832	0.000000	-2.905796	2.925226	0.000000
6	1.438652	1.606086	-1.155695	-1.464127	1.616215	1.163928
1	1.667866	1.843534	-2.189452	-1.701663	1.850380	2.205204
25	-2.422230	-0.079552	0.000000	2.400831	-0.091291	0.000000
6	-3.711316	-0.289170	1.261864	3.700588	-0.295796	-1.225296
6	-2.503210	1.733782	0.000000	2.483716	1.711969	0.000000
6	-3.711306	-0.289129	-1.261882	3.700603	-0.295761	1.225293
8	-4.543548	-0.421562	2.059803	4.573708	-0.419200	-2.004518
8	-4.543531	-0.421499	-2.059832	4.573738	-0.419135	2.004503
8	-2.520380	2.893435	0.000000	2.518709	2.885903	0.000000
25	2.464351	0.055155	0.000000	-2.447066	0.068212	0.000000
6	3.707477	-0.096905	-1.293632	-3.688157	-0.112523	1.271416
6	3.707329	-0.097091	1.293748	-3.688244	-0.112507	-1.271348
6	2.144126	-1.719425	-0.000144	-2.127594	-1.693782	0.000000
8	4.496304	-0.166042	-2.144619	-4.499908	-0.214199	2.119436
8	-1.316481	-0.166347	2.144821	-4.500063	-0.214188	-2.119302
8	-1.110462	-2.864961	-0.000238	-1.939280	-2.857739	0.000000

6S-2

	B3LYP			BP86		
	x	y	z	x	y	z
6	2.339789	2.136277	0.000000	-2.339009	-2.147111	0.000000
6	1.823063	1.703322	1.262283	-1.835550	-1.691100	1.268396
6	0.662811	0.918448	1.450578	-0.672492	-0.878737	1.443405
6	1.823052	1.703276	-1.262363	-1.835520	-1.691097	-1.268437
6	-0.581148	1.220987	0.705049	0.576713	-1.204553	0.711186
6	0.662794	0.918400	-1.450607	-0.672454	-0.878742	-1.443416
6	-0.581154	1.220972	-0.705071	0.576731	-1.204569	-0.711166
1	3.269466	2.700400	0.000000	-3.273523	-2.720629	0.000000
1	2.484035	1.861493	2.115066	-2.495322	-1.861875	2.130372
1	0.544662	0.483489	2.443113	-0.561941	-0.416664	2.433748
1	2.484015	1.861413	-2.115159	-2.495274	-1.861867	-2.130429
1	0.544624	0.483403	-2.443123	-0.561874	-0.416663	-2.433754
6	-1.834964	1.754464	1.161836	1.834219	-1.752008	1.170672
1	-2.136840	1.899773	2.192979	2.142359	-1.891851	2.209450
6	-2.598553	2.090071	0.000000	2.601459	-2.092568	0.000000
1	-3.599437	2.508967	0.000000	3.607444	-2.520800	0.000000
6	-1.834972	1.754445	-1.161858	1.834242	-1.752034	-1.170614
1	-2.136855	1.899737	-2.193002	2.142405	-1.891902	-2.209381
25	-2.246244	-0.039727	0.000000	2.243681	0.019420	0.000000
6	-1.989526	-1.241875	-1.317852	2.017831	1.227912	-1.298495
6	-4.025263	-0.326670	0.000000	4.008181	0.308476	-0.000174
8	-1.809139	-1.976726	-2.199610	1.868689	1.994063	-2.180486
8	-5.177403	-0.481622	0.000000	5.173579	0.482633	-0.000313
6	3.356821	-0.580514	1.261576	-3.362579	0.574979	1.226129
6	1.268908	-1.592336	0.000000	-1.271729	1.561633	0.000125
6	3.356832	-0.580581	-1.261555	-3.362440	0.575072	-1.226257
8	0.706788	-2.604394	0.000000	-0.718262	2.594446	0.000250
8	4.117859	-0.939148	2.060584	-4.150518	0.965904	2.007315
8	4.117894	-0.939257	-2.060522	-4.150277	0.966063	-2.007512
25	2.174935	-0.020166	0.000000	-2.177155	0.000819	0.000000
6	-1.989515	-1.241836	1.317885	2.018081	1.227812	1.298659
8	-1.809103	-1.976659	2.199662	1.869097	1.993901	2.180731

6T-3

	B3LYP			BP86		
	x	y	z	x	y	z
6	1.550294	-1.959868	-0.436022	1.530357	-1.876958	-0.551878
6	1.203708	-0.978185	-1.395040	1.188692	-0.864620	-1.507443
6	0.655881	0.295754	-1.100070	0.599590	0.388733	-1.156302
6	0.914253	-2.222241	0.858987	1.199359	-1.898465	0.846476
6	-0.319198	0.568159	-0.028739	-0.349623	0.660469	-0.076529
6	-0.081160	-1.542411	1.495569	0.136666	-1.276298	1.558907
6	-0.671954	-0.271567	1.102468	-0.600895	-0.129727	1.131188
1	2.139208	-2.792455	-0.817163	2.136627	-2.713980	-0.919459
1	1.620652	-1.112192	-2.393155	1.534638	-1.001894	-2.538628
1	0.603895	0.996253	-1.932176	0.586613	1.142273	-1.954778
1	1.276661	-3.123977	1.353270	1.734055	-2.677007	1.408143
1	-0.449187	-1.958012	2.433824	-0.053896	-1.639961	2.576600
6	-1.066301	1.773206	0.085493	-1.187806	1.829443	-0.012913
1	-1.019539	2.601771	-0.613630	-1.213688	2.626814	-0.759990
6	-1.865555	1.720080	1.276634	-1.945744	1.788640	1.214174
1	-2.517697	2.501839	1.647463	-2.649197	2.549366	1.559955
6	-1.614043	0.463557	1.894454	-1.614539	0.576168	1.895445
1	-2.055292	0.108506	2.820153	-2.005695	0.253307	2.863664
25	2.627650	-0.019898	-0.144399	2.518826	-0.016521	-0.087345
6	4.324920	-0.778255	-0.311601	4.087424	-0.710529	-0.628867
6	3.297887	1.565443	-0.847424	3.073560	1.577842	-0.719675
6	2.567577	0.734957	1.642988	3.055305	0.388864	1.622666
8	5.374630	-1.261804	-0.412509	5.121123	-1.153225	-0.981340
8	2.546639	1.227913	2.686388	3.436160	0.668351	2.698959
8	3.716038	2.559635	-1.277735	3.446906	2.618602	-1.125264
25	-2.511230	0.131754	-0.054640	-2.529749	0.111196	0.000869
6	-3.904566	-0.707617	0.721725	-3.546221	-1.155770	0.754643
6	-3.602017	1.108507	-1.105207	-3.962841	0.980026	-0.610998
6	-2.324541	-1.168133	-1.294974	-2.404147	-0.819883	-1.527840
8	-4.789991	-1.241996	1.251620	-4.212857	-1.980346	1.266942
8	-4.286331	1.768965	-1.772793	-4.902223	1.567850	-1.010314
8	-2.173524	-2.006021	-2.084728	-2.308010	-1.427905	-2.531472

6T-4

	B3LYP			BP86		
	x	y	z	x	y	z
6	3.051552	2.188025	-0.140294	0.639782	3.577363	-0.014774
6	2.038859	2.996213	0.510366	-0.517539	3.519302	0.839104
6	0.680694	2.952856	0.391321	-1.575582	2.627864	0.836594
6	2.893727	1.082223	-0.931039	1.045542	2.682223	-1.012254
6	-0.091058	2.109652	-0.502748	-1.828308	1.567908	-0.120391
6	1.697276	0.362291	-1.349262	0.385561	1.526043	-1.524290
6	0.352491	0.936923	-1.266285	-0.991880	1.153715	-1.251673
1	4.078165	2.503122	0.045104	1.329099	4.407910	0.187009
1	2.431049	3.765173	1.177850	-0.553624	4.294355	1.618119
1	0.100994	3.683137	0.956906	-2.340894	2.750218	1.615427
1	3.817204	0.639805	-1.310762	2.022196	2.891320	-1.471718
1	1.865279	-0.202553	-2.266223	0.806006	1.096818	-2.443200
6	-1.411614	2.440038	-0.933101	-3.002836	0.741797	-0.136945
1	-1.994823	3.273434	-0.554982	-3.816760	0.789923	0.591161
6	-1.809806	1.536315	-1.951586	-2.947650	-0.121738	-1.293647
1	-2.760286	1.540603	-2.474269	-3.711920	-0.841963	-1.594834
6	-0.763217	0.598070	-2.134066	-1.730035	0.146226	-1.987188
1	-0.758437	-0.204649	-2.863177	-1.380797	-0.356016	-2.893073
25	-1.473448	0.354198	-0.052623	-1.263840	-0.564720	-0.005121
6	-2.942773	-0.755015	-0.283058	-0.105502	-1.814227	-0.856801
6	-2.228260	0.796872	1.579407	-2.075460	-1.961892	0.774526
8	-3.863321	-1.446844	-0.414773	0.018091	-2.786034	-1.535860
8	-2.726891	1.079157	2.586705	-2.633150	-2.868093	1.276494
6	2.317356	-1.993728	0.300659	2.290748	0.729270	0.967992
6	-0.324591	-1.979529	1.133223	1.955102	-1.787793	0.844628
6	0.348288	-2.143939	-1.338467	2.451844	-0.587535	-1.323279
8	-0.968842	-2.660679	1.822711	2.459299	-2.696609	1.394933
8	3.289777	-2.609785	0.448428	3.011838	1.397660	1.612172
8	0.095673	-2.894756	-2.183256	3.253058	-0.728266	-2.175009
25	0.804408	-1.023104	0.070837	1.236436	-0.389862	-0.007921
6	1.283475	-0.041052	1.585874	-0.390534	-0.245391	1.600019
8	1.597661	0.433817	2.591254	-0.270101	-0.029511	2.760699

5S-1

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.650421	2.852080	0.000000	1.336076	-3.045418	0.000000
6	-1.663775	2.204033	1.272133	1.411881	-2.406307	1.278434
6	-1.554922	0.846899	1.578987	1.499050	-1.030790	1.590387
6	-1.663775	2.204033	-1.272133	1.411881	-2.406307	-1.278434
6	-1.647348	-0.314983	0.723767	1.698764	0.107343	0.731678
6	-1.554922	0.846899	-1.578987	1.499050	-1.030790	-1.590387
6	-1.647348	-0.314983	-0.723767	1.698764	0.107343	-0.731678
1	-1.659979	3.939202	0.000000	1.164774	-4.128438	0.000000
1	-1.572797	2.873614	2.126775	1.219090	-3.061136	2.138119
1	-1.354667	0.623411	2.626313	1.312537	-0.782512	2.643646
1	-1.572797	2.873614	-2.126775	1.219090	-3.061136	-2.138119
1	-1.354667	0.623411	-2.626313	1.312537	-0.782512	-2.643646
6	-1.711114	-1.680271	1.158326	1.844999	1.479910	1.165260
1	-1.757082	-2.008800	2.190432	1.910326	1.806843	2.205577
6	-1.782366	-2.510848	0.000000	1.985427	2.307983	0.000000
1	-1.905673	-3.588017	0.000000	2.205547	3.377857	0.000000
6	-1.711114	-1.680271	-1.158326	1.844999	1.479910	-1.165260
1	-1.757082	-2.008800	-2.190432	1.910326	1.806843	-2.205577
25	0.000000	1.526007	0.000000	-0.089762	-1.479798	0.000000
6	1.212880	2.065405	1.216139	-1.387473	-1.850618	1.166582
6	1.268322	-1.110209	-1.346926	-1.150309	1.226507	-1.342230
6	1.212880	2.065405	-1.216139	-1.387473	-1.850618	-1.166582
8	2.014214	2.483458	1.950788	-2.282160	-2.170492	1.867862
8	2.014214	2.483458	-1.950788	-2.282160	-2.170492	-1.867862
8	1.965501	-0.893263	-2.249070	-1.883773	1.111415	-2.254826
25	0.145502	-1.573167	0.000000	0.006495	1.543604	0.000000
6	0.841898	-3.228096	0.000000	-0.531624	3.239348	0.000000
6	1.268322	-1.110209	1.346926	-1.150309	1.226507	1.342230
8	1.289844	-4.300136	0.000000	-0.907479	4.356284	0.000000
8	1.965501	-0.893263	2.249070	-1.883773	1.111415	2.254826

5S-2

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.741272	-1.940646	-0.988655	-1.768867	-1.882477	-1.090331
6	-1.704690	-2.126302	0.430955	-1.771646	-2.135886	0.325877
6	-0.637782	-1.716587	1.253178	-0.713679	-1.757436	1.196272
6	-0.712571	-1.359282	-1.763102	-0.704138	-1.264155	-1.808460
6	0.773054	-1.636909	0.928740	0.706728	-1.666044	0.902490
6	0.716619	-1.355174	-1.549189	0.732239	-1.320286	-1.577096
6	1.404316	-1.819512	-0.385927	1.379196	-1.840399	-0.402882
1	-2.681630	-2.157248	-1.490895	-2.708697	-2.055149	-1.628669
1	-2.622145	-2.455956	0.913773	-2.711152	-2.479158	0.775241
1	-0.856641	-1.664020	2.319922	-0.960405	-1.740978	2.266727
1	-1.010297	-1.065309	-2.769322	-0.979550	-0.904422	-2.809035
1	1.314491	-1.211611	-2.448195	1.356317	-1.178545	-2.469229
6	1.771877	-1.120420	1.797279	1.690026	-1.142078	1.806638
1	1.606795	-0.811504	2.824727	1.492471	-0.829350	2.836002
6	3.011858	-1.006654	1.086911	2.956140	-1.031310	1.129617
1	3.946790	-0.647271	1.501425	3.884876	-0.663579	1.571657
6	2.805557	-1.470967	-0.238784	2.786576	-1.495065	-0.213631
1	3.544374	-1.500812	-1.032221	3.551447	-1.521421	-0.993926
25	-1.504354	-0.011958	-0.044817	-1.481902	-0.031725	-0.049604
6	-3.260958	0.246998	-0.268379	-3.203661	0.332404	-0.302846
6	-1.561303	0.935688	1.497897	-1.584623	0.848393	1.515527
6	-1.117511	1.414810	-1.097327	-1.023809	1.413593	-1.030792
8	-4.399898	0.437435	-0.406401	-4.339252	0.609217	-0.456225
8	-0.932833	2.310589	-1.814230	-0.834773	2.346756	-1.722727
8	-1.635558	1.499884	2.510202	-1.700942	1.392467	2.552459
25	1.499896	0.138068	0.026736	1.482773	0.111876	0.035749
6	2.249761	1.128653	-1.279050	2.298340	1.120010	-1.190374
6	1.331243	1.688065	0.977673	1.318977	1.667514	0.950942
8	2.788232	1.734255	-2.114556	2.895812	1.758421	-1.984212
8	1.292623	2.666637	1.602420	1.287419	2.679157	1.552191

5S-3

	B3LYP			BP86		
	x	y	z	x	y	z
6	1.110742	0.896494	-1.751374	-1.133761	0.307884	-1.966138
6	0.925559	1.735352	-0.602299	-0.929120	-1.041042	-1.520318
6	0.386394	1.361658	0.634478	-0.411716	-1.465142	-0.261055
6	0.893668	-0.513837	-1.750281	-0.942345	1.462387	-1.132021
6	-0.674215	0.361717	0.870150	0.635468	-0.809860	0.538163
6	0.430436	-1.309691	-0.676249	-0.401341	1.490039	0.182246
6	-0.621000	-0.940767	0.291156	0.652564	0.623177	0.733688
1	1.539037	1.343118	-2.645112	-1.586635	0.457239	-2.952822
1	1.392888	2.717806	-0.666573	-1.348430	-1.820035	-2.170876
1	0.534744	2.082203	1.439435	-0.555837	-2.534022	-0.051237
1	1.298021	-1.041189	-2.614591	-1.383517	2.394580	-1.508866
1	0.570202	-2.381821	-0.814081	-0.548577	2.440947	0.713148
6	-1.787807	0.390868	1.765537	1.723390	-1.376377	1.267408
1	-2.095063	1.235503	2.373651	1.978579	-2.438328	1.318186
6	-2.437475	-0.881707	1.712727	2.459514	-0.292157	1.885327
1	-3.299292	-1.184785	2.295281	3.341298	-0.392171	2.521456
6	-1.681246	-1.719699	0.809762	1.760256	0.937691	1.583447
1	-1.894777	-2.754737	0.565261	2.045694	1.937050	1.923186
25	2.232547	0.034447	-0.131382	-2.217877	0.014933	-0.146579
6	3.549227	1.246206	0.185643	-3.500293	-1.186926	-0.509678
6	2.327034	-0.732925	1.511559	-2.302127	-0.235029	1.640039
6	3.488705	-1.045784	-0.869039	-3.524388	1.246174	-0.174528
8	4.399545	2.010508	0.385340	-4.364293	-1.952003	-0.740538
8	4.300130	-1.729611	-1.339374	-4.403681	2.028228	-0.192349
8	2.353606	-1.227360	2.559933	-2.340787	-0.399653	2.802070
25	-2.522422	0.018260	-0.220743	2.488271	0.005981	-0.196674
6	-3.956181	-0.887268	-0.823959	3.601682	1.366910	-0.483890
6	-3.384456	1.596556	-0.234507	3.744484	-1.149765	-0.711622
8	-4.892420	-1.509511	-1.133851	4.352650	2.275069	-0.599388
8	-3.937762	2.621373	-0.168297	4.594106	-1.931130	-0.974454

5T-4

	B3LYP			BP86		
	x	y	z	x	y	z
6	2.125795	-2.540579	0.000000	2.112860	-2.602094	0.000000
6	1.692175	-2.028983	1.257686	1.699233	-2.077133	1.266899
6	0.932238	-0.836402	1.444690	0.979628	-0.846007	1.457260
6	1.692175	-2.028983	-1.257686	1.699233	-2.077133	-1.266899
6	1.249869	0.409181	0.707050	1.308939	0.390169	0.715112
6	0.932238	-0.836402	-1.444690	0.979628	-0.846007	-1.457260
6	1.249869	0.409181	-0.707050	1.308939	0.390169	-0.715112
1	2.636143	-3.501979	0.000000	2.577177	-3.596625	0.000000
1	1.835462	-2.690432	2.113385	1.817156	-2.746973	2.130148
1	0.522982	-0.703983	2.446504	0.558593	-0.704485	2.461932
1	1.835462	-2.690432	-2.113385	1.817156	-2.746973	-2.130148
1	0.522982	-0.703983	-2.446504	0.558593	-0.704485	-2.461932
6	1.704784	1.693148	1.162473	1.720359	1.698670	1.171048
1	1.827734	2.006127	2.193236	1.826402	2.020723	2.209561
6	1.987306	2.478146	0.000000	1.981002	2.496015	0.000000
1	2.342270	3.503530	0.000000	2.313654	3.537470	0.000000
6	1.704784	1.693148	-1.162473	1.720359	1.698670	-1.171048
1	1.827734	2.006127	-2.193236	1.826402	2.020723	-2.209561
25	-0.073444	-2.205304	0.000000	-0.031363	-2.168642	0.000000
6	-1.154114	-2.810922	1.395080	-1.196061	-2.692439	1.304713
6	-1.297907	1.612406	-1.306380	-1.272734	1.570086	-1.289823
6	-1.154114	-2.810922	-1.395080	-1.196061	-2.692439	-1.304713
8	-1.802625	-3.162862	2.287522	-1.948139	-3.033023	2.142886
8	-1.802625	-3.162862	-2.287522	-1.948139	-3.033023	-2.142886
8	-2.029808	1.349172	-2.171248	-2.034272	1.331665	-2.156512
25	-0.115874	1.979424	0.000000	-0.086365	1.927202	0.000000
6	-0.539133	3.732876	0.000000	-0.552931	3.654291	0.000000
6	-1.297907	1.612406	1.306380	-1.272734	1.570086	1.289823
8	-0.783406	4.869659	0.000000	-0.843914	4.796117	0.000000
8	-2.029808	1.349172	2.171248	-2.034272	1.331665	2.156512

5T-5

	B3LYP			BP86		
	x	y	z	x	y	z
6	-2.046570	1.783707	0.492655	-2.004034	1.852595	0.473937
6	-2.278909	1.453645	-0.890531	-2.253344	1.491590	-0.907144
6	-1.253186	1.007166	-1.736318	-1.222084	1.049197	-1.768730
6	-1.024477	2.742580	0.957585	-0.964604	2.795836	0.930184
6	0.163653	1.072663	-1.368215	0.199649	1.097192	-1.406301
6	0.255116	2.861877	0.533286	0.330852	2.887279	0.504184
6	0.854141	1.970728	-0.450678	0.911593	1.968994	-0.464334
1	-2.964636	1.845930	1.077245	-2.919596	1.909366	1.078265
1	-3.301164	1.384885	-1.261061	-3.287993	1.407729	-1.264762
1	-1.490272	0.692320	-2.750107	-1.472322	0.703597	-2.778826
1	-1.357296	3.421499	1.744888	-1.281899	3.480600	1.730703
1	0.905099	3.612049	0.981461	1.004422	3.619272	0.967970
6	1.201405	0.368267	-2.100011	1.218404	0.307443	-2.089490
1	1.018185	-0.354979	-2.888414	1.014345	-0.428436	-2.872322
6	2.470814	0.863703	-1.699685	2.510314	0.684413	-1.600615
1	3.433492	0.547238	-2.085506	3.470524	0.277852	-1.926197
6	2.253840	1.829848	-0.679906	2.315099	1.690667	-0.600504
1	3.024690	2.368145	-0.136879	3.101699	2.171298	-0.011340
25	-1.394463	-0.266840	-0.034875	-1.339955	-0.206182	-0.043678
6	-3.011161	-0.992852	0.280480	-2.885943	-0.940331	0.487142
6	-0.991632	-1.796831	-0.934776	-1.108095	-1.718599	-1.012549
6	-0.889012	-0.644200	1.667330	-0.668889	-0.579389	1.609273
8	-4.054569	-1.461080	0.488286	-3.883734	-1.445304	0.856423
8	-0.673196	-0.862232	2.790237	-0.460227	-0.827523	2.745888
8	-0.819018	-2.787605	-1.521490	-1.055425	-2.710994	-1.647494
25	1.415148	-0.186344	-0.002834	1.302052	-0.191059	-0.001208
6	2.261101	-0.149035	1.652887	2.264324	-0.226511	1.540469
6	2.157084	-1.866395	-0.183563	1.850234	-1.905518	-0.187490
8	2.832389	-0.131159	2.659516	2.943952	-0.254416	2.498744
8	2.649586	-2.910013	-0.289317	2.250127	-3.004187	-0.309751

5T-6

	B3LYP			BP86		
	x	y	z	x	y	z
6	1.019676	1.731227	0.807985	0.958537	1.658382	0.955517
6	0.786015	0.628662	1.690359	0.760963	0.466612	1.732658
6	0.301416	-0.645288	1.346138	0.319591	-0.798847	1.249643
6	0.896512	1.653757	-0.613475	0.876234	1.698739	-0.478076
6	-0.717032	-0.947474	0.321501	-0.709625	-1.018607	0.212782
6	0.435916	0.551163	-1.356704	0.444141	0.633531	-1.315453
6	-0.667114	-0.354622	-0.968029	-0.675783	-0.291762	-1.015713
1	1.427506	2.644411	1.234121	1.349332	2.543500	1.470672
1	1.184450	0.753596	2.697447	1.134057	0.512196	2.764873
1	0.417036	-1.404723	2.119836	0.460318	-1.631390	1.952780
1	1.360141	2.472913	-1.163425	1.330321	2.578439	-0.953905
1	0.634590	0.601426	-2.427278	0.673093	0.760974	-2.382324
6	-1.798564	-1.865868	0.352405	-1.812402	-1.928687	0.174434
1	-2.083797	-2.498454	1.186335	-2.100799	-2.632923	0.959026
6	-2.418959	-1.856209	-0.956932	-2.458499	-1.782663	-1.120609
1	-3.238358	-2.491022	-1.274376	-3.310190	-2.367062	-1.476887
6	-1.693771	-0.932661	-1.772979	-1.741843	-0.770747	-1.858218
1	-1.893204	-0.696400	-2.813384	-1.960191	-0.426436	-2.872887
25	2.177092	0.048468	0.109461	2.142303	0.061660	0.126714
6	3.411637	-0.254690	1.407714	3.378992	-0.348393	1.368062
6	2.294071	-1.612681	-0.611649	2.286763	-1.506540	-0.755310
6	3.511110	0.747814	-0.904258	3.490846	0.855898	-0.758698
8	4.208251	-0.447680	2.229817	4.210572	-0.615301	2.156849
8	4.371725	1.190502	-1.545349	4.395554	1.356902	-1.320497
8	2.335468	-2.674676	-1.075740	2.362454	-2.527062	-1.331015
25	-2.699437	0.080243	-0.078493	-2.660122	0.054093	-0.086282
6	-2.604756	1.922438	-0.220174	-2.683910	1.866507	-0.263720
6	-4.323592	-0.177247	0.738741	-4.144453	-0.205737	0.918778
8	-2.492952	3.072036	-0.349845	-2.658511	3.036501	-0.416229
8	-5.340632	-0.406364	1.253952	-5.106041	1.658382	1.567315

4T-1

	B3LYP			BP86		
	x	y	z	x	y	z
6	2.003118	1.821270	-0.240211	-1.808614	-2.118393	0.126618
6	1.955259	1.302037	1.090243	-1.667699	-1.332161	1.312323
6	0.792901	0.789984	1.699306	-0.479653	-0.660734	1.727207
6	1.053510	2.748577	-0.859760	-0.819805	-2.867480	-0.621114
6	-0.565017	1.005600	1.192030	0.866979	-0.892445	1.217099
6	-0.286406	2.847766	-0.666246	0.557560	-2.788457	-0.582062
6	-1.059657	1.936736	0.165971	1.333905	-1.818123	0.172685
1	3.016552	1.931645	-0.626464	-2.847629	-2.376861	-0.118099
1	2.893692	1.151754	1.622375	-2.565655	-1.176951	1.922764
1	0.870012	0.364291	2.697983	-0.534578	-0.070671	2.650956
1	1.496459	3.426699	-1.591428	-1.244738	-3.573952	-1.347783
1	-0.852546	3.587740	-1.230212	1.129313	-3.443251	-1.253396
6	-1.713933	0.298609	1.696865	1.986588	-0.045512	1.571724
1	-1.693476	-0.449177	2.483137	1.966932	0.744447	2.326507
6	-2.876112	0.764858	1.010919	3.125441	-0.434612	0.773681
1	-3.893415	0.432414	1.185540	4.120725	0.013334	0.818104
6	-2.470567	1.785945	0.102592	2.722035	-1.522509	-0.062288
1	-3.119638	2.325866	-0.580423	3.343857	-2.022053	-0.811812
25	1.263817	-0.344085	-0.032104	-1.254870	0.221635	-0.077372
6	2.957443	-0.980279	-0.100200	-3.005567	0.595280	-0.194032
6	0.795286	-1.898060	0.748812	-1.095189	1.785703	0.752512
8	4.040374	-1.397051	-0.156672	-4.143562	0.888317	-0.285673
8	0.574645	-2.881802	1.337528	-1.044290	2.802116	1.352923
25	-1.467715	-0.203631	-0.379368	1.475936	0.283236	-0.459201
6	-0.130121	-0.426965	-1.618575	0.144830	0.334305	-1.644128
6	-2.483781	-1.747052	-0.650976	1.891731	2.033727	-0.592259
8	0.835487	-0.596026	-2.287999	-0.932528	0.347688	-2.217717
8	-3.131973	-2.696680	-0.780148	2.194116	3.170962	-0.664622

4S-2

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.471690	-2.038108	0.827605	1.637236	2.065152	0.783485
6	-1.325354	-1.032489	1.827925	1.444822	1.099570	1.822594
6	-0.752293	0.254824	1.703572	0.772184	-0.157307	1.759586
6	-1.216377	-1.979926	-0.576922	1.362320	1.971813	-0.619883
6	0.180813	0.641180	0.649779	-0.147407	-0.563386	0.712301
6	-0.589255	-0.941386	-1.294110	0.644807	0.947324	-1.298354
6	0.275767	0.070357	-0.692309	-0.237663	-0.018415	-0.663481
1	-2.130131	-2.854167	1.121572	2.366850	2.844576	1.040120
1	-1.868958	-1.230174	2.751042	2.022454	1.288985	2.736688
1	-0.819771	0.927683	2.555498	0.825499	-0.808880	2.640202
1	-1.690816	-2.765139	-1.163425	1.882576	2.706163	-1.247617
1	-0.545744	-1.020898	-2.378134	0.603191	0.989675	-2.393465
6	1.060512	1.772343	0.707062	-1.052915	-1.690993	0.795187
1	1.185093	2.420742	1.566953	-1.192805	-2.314584	1.681500
6	1.698488	1.910668	-0.565075	-1.707987	-1.845469	-0.472110
1	2.428789	2.667373	-0.829733	-2.451717	-2.606561	-0.719946
6	1.233610	0.875708	-1.416190	-1.232541	-0.821758	-1.357498
1	1.514339	0.716156	-2.451327	-1.518916	-0.681021	-2.402639
25	-2.002315	-0.066172	0.019189	1.999987	0.024824	0.032518
6	-2.419671	1.541852	-0.685147	2.367453	-1.587271	-0.651663
6	-3.767049	-0.345872	0.055292	3.764026	0.157372	0.030973
8	-4.925252	-0.479979	0.056842	4.946505	0.181216	0.001764
8	-2.768588	2.558227	-1.135671	2.709963	-2.625808	-1.099179
25	2.254970	0.009587	0.273763	-2.202388	0.057704	0.292416
6	2.809187	-1.474385	-0.591032	-2.743293	1.520704	-0.579516
6	3.929929	0.604174	0.562235	-3.883816	-0.483999	0.489011
8	3.136203	-2.398506	-1.219529	-3.087276	2.446376	-1.229444
8	5.000563	1.038828	0.709798	-4.994250	-0.881982	0.581610

4T-3

	B3LYP			BP86		
	x	y	z	x	y	z
6	1.378490	1.995821	0.904283	-1.422103	2.054979	0.861825
6	1.162088	0.963018	1.866261	-1.282464	1.991276	-0.562662
6	0.606412	-0.318136	1.658335	-0.708812	0.944222	-1.339502
6	1.239487	1.969054	-0.515852	-1.188031	1.047886	1.853782
6	-0.222613	-0.684524	0.515656	0.194760	-0.075597	-0.824559
6	0.705931	0.934984	-1.314910	-0.586639	-0.234166	1.686477
6	-0.204956	-0.096214	-0.821373	0.213658	-0.641011	0.545647
1	1.995969	2.814641	1.270480	-2.074441	2.868467	1.205752
1	1.620730	1.141190	2.837890	-1.818425	2.772683	-1.116445
1	0.601761	-1.013839	2.494587	-0.780346	1.019293	-2.431243
1	1.749875	2.776069	-1.039729	-1.661263	1.237852	2.825630
1	0.764220	1.043847	-2.395656	-0.580178	-0.911942	2.548681
6	-1.102154	-1.812701	0.464302	1.039635	-0.929280	-1.642841
1	-1.323798	-2.458582	1.307073	1.198264	-0.786976	-2.714983
6	-1.581734	-1.974441	-0.871583	1.572425	-1.978634	-0.825954
1	-2.262752	-2.748220	-1.209683	2.255490	-2.768408	-1.149527
6	-1.044812	-0.921440	-1.658605	1.089920	-1.787911	0.512941
1	-1.193787	-0.761364	-2.721084	1.317130	-2.415758	1.378075
25	2.012352	0.053608	0.104358	-1.975490	0.065668	0.106423
6	2.508876	-1.546932	-0.561155	-2.482780	-1.524724	-0.533750
6	3.762281	0.366910	0.271406	-3.720287	0.300223	0.250769
8	4.914729	0.523046	0.361049	-4.897800	0.394593	0.323492
8	2.906959	-2.558711	-0.981769	-2.911791	-2.546761	-0.944662
25	-2.323414	-0.058853	-0.109776	2.289655	-0.081911	-0.110195
6	-2.763877	1.596721	-0.791978	3.720825	-0.443755	0.957530
6	-3.753034	-0.427087	1.007783	2.771858	1.546743	-0.762536
8	-2.984927	2.636182	-1.259632	4.636102	-0.726421	1.643989
8	-4.626510	-0.717118	1.714871	3.050721	2.599755	-1.212150

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	B3LYP			BP86		
	x	y	z	x	y	z
6	1.710105	-2.086127	0.015711	-1.623040	2.365368	-0.313572
6	1.676053	-1.409986	-1.247339	-1.564637	1.358014	-1.329040
6	0.568369	-0.689406	-1.736931	-0.435015	0.563397	-1.705884
6	0.685284	-2.941942	0.589346	-0.583972	3.065683	0.367380
6	-0.772460	-0.781005	-1.148061	0.916093	0.718861	-1.171626
6	-0.667188	-2.868008	0.449581	0.787347	2.821547	0.392652
6	-1.346850	-1.793738	-0.243384	1.464843	1.719761	-0.223605
1	2.717637	-2.360829	0.328120	-2.638142	2.732054	-0.108459
1	2.595479	-1.351479	-1.828655	-2.474806	1.217769	-1.925670
1	0.643354	-0.192223	-2.702005	-0.523046	-0.052270	-2.610066
1	1.065265	-3.726717	1.246453	-0.932648	3.890990	1.004324
1	-1.297029	-3.582655	0.977493	1.402908	3.463900	1.036979
6	-1.857394	0.090131	-1.527939	2.000301	-0.190352	-1.497759
1	-1.759712	0.928133	-2.210854	1.919367	-1.031612	-2.191012
6	-3.058496	-0.338801	-0.892679	3.154012	0.166055	-0.724771
1	-4.041831	0.099480	-1.019761	4.109247	-0.365318	-0.730017
6	-2.725895	-1.487569	-0.101035	2.818763	1.307356	0.083952
1	-3.411982	-2.044345	0.532366	3.484306	1.832964	0.774931
25	1.274603	0.203352	0.029442	-1.214703	-0.195185	0.094470
6	3.050274	0.488403	0.123113	-2.992858	-0.374057	0.203131
6	1.114119	1.884392	-0.587061	-1.223530	-1.804659	-0.606440
8	4.195895	0.680577	0.181437	-4.156377	-0.548565	0.278057
8	1.091274	2.944318	-1.074320	-1.300825	-2.864806	-1.127903
25	-1.619782	0.274955	0.573525	1.507232	-0.342676	0.545533
6	-0.165511	0.290703	1.656969	0.153505	-0.198406	1.717293
6	-1.781543	2.081868	0.498612	1.530435	-2.138990	0.476591
8	0.838381	0.350993	2.287729	-0.931814	-0.089310	2.261662
8	-1.932412	3.229046	0.015711	1.629780	-3.312247	0.430569

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	B3LYP			BP86		
	x	y	z	x	y	z
6	-2.300108	-1.544230	0.862765	-2.302481	-1.523029	0.865984
6	-1.227313	-1.229615	1.741714	-1.212111	-1.183847	1.742257
6	0.199268	-1.275925	1.514627	0.217644	-1.285345	1.516169
6	-2.230314	-1.583251	-0.559093	-2.236290	-1.596695	-0.555809
6	0.895478	-1.722484	0.324395	0.913089	-1.752974	0.325199
6	-1.085435	-1.299651	-1.345505	-1.075931	-1.316260	-1.353637
6	0.324828	-1.443244	-0.998399	0.334232	-1.462698	-1.004442
1	-3.297619	-1.552078	1.297925	-3.307002	-1.506626	1.307572
1	-1.514012	-0.992326	2.766029	-1.494857	-0.911441	2.768243
1	0.807471	-1.163906	2.409810	0.837029	-1.157405	2.413207
1	-3.184511	-1.597541	-1.083653	-3.197728	-1.614680	-1.085511
1	-1.272485	-1.090778	-2.399252	-1.264533	-1.098123	-2.414596
6	2.319215	-1.512864	0.228256	2.342906	-1.495987	0.234330
1	3.019951	-1.618078	1.049024	3.046249	-1.590111	1.065561
6	2.623055	-1.056825	-1.088906	2.641004	-1.001968	-1.078433
1	3.607260	-0.800236	-1.464082	3.625642	-0.703212	-1.444991
6	1.411218	-0.990958	-1.827342	1.419470	-0.948363	-1.823696
1	1.313261	-0.664054	-2.857488	1.312000	-0.596717	-2.853464
25	-1.232922	0.158713	0.161237	-1.209103	0.134512	0.132302
6	-2.594505	1.306867	0.027982	-2.534203	1.272688	0.018995
8	-3.459976	2.085486	-0.047297	-3.395764	2.087027	-0.056409
25	1.162970	0.260581	-0.034973	1.142054	0.242813	-0.029192
6	0.491619	1.752281	-0.791865	0.413031	1.733365	-0.738100
6	2.164649	1.324337	1.018108	2.125904	1.331579	0.997199
8	0.174977	2.740375	-1.336613	0.096872	2.751213	-1.261627
8	2.824944	2.005393	1.694494	2.779125	2.052061	1.666802

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	B3LYP			BP86		
	x	y	z	x	y	z
6	2.187687	-1.516622	0.974809	2.142176	-1.513361	1.049914
6	2.117195	-1.588247	-0.451164	2.141266	-1.594893	-0.381168
6	0.978676	-1.283739	-1.227145	1.018712	-1.265893	-1.209743
6	1.124564	-1.118784	1.831737	1.041989	-1.056213	1.844064
6	-0.440453	-1.427372	-0.873515	-0.412290	-1.424253	-0.906305
6	-0.285536	-1.084968	1.621940	-0.377649	-1.075996	1.594220
6	-1.011345	-1.545200	0.470929	-1.043051	-1.579892	0.421565
1	3.171871	-1.620872	1.426312	3.114941	-1.599441	1.549629
1	3.062015	-1.712811	-0.977532	3.108317	-1.760685	-0.872383
1	1.159492	-1.146113	-2.293073	1.240992	-1.126103	-2.276496
1	1.438355	-0.816554	2.832465	1.317653	-0.707752	2.850616
1	-0.883481	-0.839269	2.498205	-1.015344	-0.863320	2.462437
6	-1.522500	-1.088653	-1.739851	-1.462641	-0.993269	-1.792432
1	-1.420303	-0.838722	-2.791662	-1.307379	-0.672871	-2.827324
6	-2.739270	-1.040634	-0.999988	-2.714596	-0.939239	-1.091199
1	-3.723260	-0.840028	-1.407881	-3.680690	-0.671150	-1.524377
6	-2.432853	-1.339272	0.366645	-2.467989	-1.322819	0.273344
1	-3.134041	-1.365816	1.193481	-3.201683	-1.361340	1.082708
25	1.426376	0.317000	0.208892	1.417175	0.296533	0.194981
6	2.974794	1.163717	-0.078791	2.948977	1.132686	-0.077995
6	0.343332	1.362799	-0.779470	0.361212	1.367655	-0.764719
8	3.965661	1.747594	-0.266691	3.950740	1.737044	-0.264769
8	-0.465917	1.839868	-1.527110	-0.479657	1.855414	-1.501614
25	-1.308733	0.359738	-0.110457	-1.274347	0.338686	-0.093714
6	-2.328058	1.517533	0.837694	-2.293822	1.458591	0.872116
8	-3.050884	2.187338	1.460780	-3.026240	2.122988	1.520574

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	B3LYP			BP86		
	x	y	z	x	y	z
6	-2.067631	2.090520	0.808724	-2.171552	2.091812	0.720691
6	-1.728912	2.053918	-0.581769	-1.785407	2.036136	-0.661860
6	-0.974047	1.073549	-1.270151	-0.961724	1.062705	-1.306873
6	-1.844753	1.130500	1.845046	-1.916264	1.183810	1.806305
6	-0.154814	0.047514	-0.658321	-0.157327	0.048466	-0.663398
6	-1.131069	-0.094515	1.781794	-1.130182	-0.011117	1.811458
6	-0.247822	-0.507613	0.710277	-0.271732	-0.481611	0.747146
1	-2.819064	2.838165	1.059116	-2.969152	2.816349	0.931125
1	-2.228098	2.801139	-1.197047	-2.304079	2.745242	-1.319957
1	-0.902514	1.160049	-2.353329	-0.888936	1.109380	-2.402032
1	-2.419118	1.300937	2.754888	-2.521705	1.358916	2.705161
1	-1.170127	-0.745876	2.653429	-1.176359	-0.640143	2.710777
6	0.772413	-0.806356	-1.381292	0.806062	-0.816104	-1.339817
1	1.038591	-0.673921	-2.423883	1.098304	-0.707445	-2.387064
6	1.182147	-1.865237	-0.532577	1.194610	-1.873978	-0.451910
1	1.867314	-2.660883	-0.805200	1.883197	-2.686077	-0.698780
6	0.598610	-1.678740	0.752564	0.581650	-1.663100	0.821575
1	0.714291	-2.326115	1.614523	0.697828	-2.289533	1.709580
25	-2.255906	0.054473	0.019700	-2.199240	0.018976	0.000429
6	-2.895009	-1.474607	-0.635598	-2.801501	-1.493225	-0.627788
8	-3.437203	-2.427098	-1.051300	-3.349188	-2.470697	-1.038870
25	1.854196	0.011817	0.281161	1.817200	0.003695	0.302642
6	3.523852	-0.629170	0.453197	3.484229	-0.588060	0.403043
6	2.416177	1.517060	-0.541000	2.397322	1.501572	-0.487058
8	4.592207	-1.089914	0.528495	4.589147	-1.013711	0.436982
8	2.753324	2.455552	-1.143367	2.775389	2.452246	-1.079946

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	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.022666	-2.092338	0.675963	-1.033317	-2.116067	0.678989
6	-1.004363	-1.157225	1.753655	-1.001478	-1.182055	1.765560
6	-0.494183	0.160967	1.757281	-0.457032	0.137379	1.782317
6	-0.678663	-1.916612	-0.698601	-0.690304	-1.937210	-0.700911
6	0.492773	0.664686	0.804626	0.493706	0.663324	0.815857
6	-0.073376	-0.794579	-1.301752	-0.063762	-0.809937	-1.306665
6	0.693519	0.214079	-0.578562	0.705776	0.197528	-0.593127
1	-1.651597	-2.961614	0.862978	-1.684385	-2.980858	0.863451
1	-1.599344	-1.449032	2.618252	-1.603616	-1.468680	2.637463
1	-0.658184	0.769062	2.644325	-0.625744	0.746441	2.679033
1	-1.068328	-2.681446	-1.368691	-1.101015	-2.694044	-1.381224
1	0.038687	-0.795170	-2.383735	0.022463	-0.801829	-2.399980
6	1.290783	1.850777	0.992092	1.290025	1.868520	0.986763
1	1.320277	2.442996	1.900675	1.333890	2.460313	1.905692
6	1.989928	2.115948	-0.224229	2.019247	2.112349	-0.227199
1	2.710453	2.913956	-0.380944	2.752056	2.910588	-0.385522
6	1.632074	1.135462	-1.186202	1.658797	1.117594	-1.195627
1	1.978163	1.078737	-2.212050	2.025858	1.045626	-2.222506
25	-1.610178	-0.094800	-0.022279	-1.571697	-0.101658	-0.006798
6	-2.071547	1.546126	-0.605891	-2.053580	1.513959	-0.597659
6	-3.352636	-0.468656	-0.139881	-3.304360	-0.418784	-0.149396
8	-4.499475	-0.662829	-0.234449	-4.473318	-0.569936	-0.264344
8	-2.447519	2.583008	-0.985124	-2.464511	2.550687	-0.991795
25	2.538885	0.184039	0.495840	2.483233	0.201571	0.480851
6	3.173099	-1.237937	-0.408059	3.115426	-1.226070	-0.394596
8	3.479961	-2.129260	-1.100737	3.439983	-2.135571	-1.085559

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	B3LYP			BP86		
	x	y	z	x	y	z
6	-2.095924	-1.566726	0.036928	-2.060403	-1.572539	0.018630
6	-1.754114	-1.104389	1.360032	-1.761763	-1.079306	1.354792
6	-0.455388	-0.702500	1.724677	-0.460643	-0.646148	1.726930
6	-1.282982	-2.393297	-0.863836	-1.226035	-2.438547	-0.832154
6	0.803263	-1.022679	1.083520	0.814054	-0.978437	1.115963
6	0.070296	-2.485359	-0.960738	0.139454	-2.527450	-0.898952
6	1.043592	-1.747295	-0.159273	1.087432	-1.744358	-0.106388
1	-3.167314	-1.687011	-0.122191	-3.136020	-1.690631	-0.172380
1	-2.555833	-0.945501	2.077992	-2.583945	-0.928147	2.064411
1	-0.358242	-0.171585	2.672989	-0.383669	-0.065299	2.657961
1	-1.862614	-2.962858	-1.591537	-1.792131	-3.037117	-1.560577
1	0.486080	-3.119265	-1.743684	0.580110	-3.186211	-1.659503
6	2.051291	-0.436759	1.483287	2.047905	-0.328697	1.499650
1	2.202864	0.160459	2.375907	2.173420	0.314814	2.374109
6	3.047525	-0.776758	0.514522	3.066193	-0.668153	0.537124
1	4.094994	-0.501346	0.554618	4.107579	-0.340074	0.563624
6	2.420900	-1.586246	-0.481769	2.469887	-1.537635	-0.437994
1	2.900301	-1.997696	-1.364949	2.968192	-1.960037	-1.315842
25	-1.325423	0.435182	0.000000	-1.316111	0.393006	-0.025665
6	-2.979271	1.106762	0.247189	-2.936382	1.063472	0.243196
8	-4.048353	1.539699	0.415338	-4.001879	1.536910	0.450885
25	1.452715	0.423819	-0.378982	1.427827	0.412441	-0.385992
6	0.134702	0.935054	-1.453439	0.107135	0.871021	-1.473961
6	1.909090	2.116472	0.044773	1.820177	2.116246	0.004046
8	-0.970175	1.228920	-1.875794	-1.013812	1.182271	-1.894107
8	2.218475	3.197893	0.355496	2.094629	3.228282	0.297516

3T-6

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.660367	2.049053	0.957210	-1.781052	2.051152	0.972499
6	-1.499592	2.020695	-0.463221	-1.594601	2.026314	-0.449742
6	-1.036417	0.930622	-1.243232	-1.057696	0.944517	-1.218942
6	-1.538925	0.960910	1.875386	-1.622823	0.971246	1.903495
6	-0.114658	-0.112519	-0.768417	-0.110537	-0.063639	-0.726483
6	-1.113336	-0.368307	1.595558	-1.119068	-0.349447	1.643503
6	-0.180966	-0.747901	0.525572	-0.182963	-0.714826	0.578389
1	-2.133701	2.945090	1.358091	-2.344933	2.912820	1.356239
1	-1.915953	2.873374	-1.000417	-2.054700	2.854174	-1.006839
1	-1.108581	1.041663	-2.324259	-1.121797	1.043484	-2.310773
1	-1.972780	1.135217	2.860814	-2.097865	1.124544	2.882970
1	-1.228152	-1.091797	2.401321	-1.222236	-1.077120	2.459402
6	0.853931	-0.839412	-1.547682	0.905881	-0.764222	-1.487679
1	1.128232	-0.614048	-2.572890	1.192529	-0.532830	-2.516743
6	1.376200	-1.894522	-0.753839	1.435069	-1.829195	-0.678152
1	2.125486	-2.614521	-1.062635	2.202818	-2.543804	-0.983488
6	0.738248	-1.838737	0.534116	0.754372	-1.805691	0.596363
1	0.902943	-2.520205	1.361561	0.917336	-2.488673	1.433589
25	-2.629360	0.305801	0.150464	-2.542293	0.220684	0.141810
6	-3.263946	-1.243358	-0.608507	-3.162233	-1.298785	-0.650259
8	-3.658289	-2.230092	-1.091567	-3.606424	-2.270597	-1.156753
25	1.871274	-0.002766	0.189285	1.854345	0.016444	0.220606
6	3.486755	-0.548669	0.775228	3.489971	-0.542122	0.640818
6	2.591460	1.396450	-0.707121	2.498300	1.414026	-0.678373
8	4.528716	-0.948822	1.112490	4.572739	-0.962647	0.871549
8	3.045115	2.264352	-1.338625	2.910165	2.301148	-1.345717

3T-7

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.390521	2.215338	0.364033	-1.203000	2.226767	-0.077343
6	-1.684774	1.618864	-0.893840	-1.531014	1.436065	-1.224613
6	-0.807981	0.784675	-1.635410	-0.678713	0.404552	-1.743107
6	-0.103608	2.656481	0.880267	0.097820	2.792954	0.291925
6	0.610840	0.600395	-1.434081	0.746392	0.237414	-1.484306
6	1.153460	2.272917	0.508581	1.352171	2.307774	0.025179
6	1.479760	1.214031	-0.442480	1.623690	1.021015	-0.613960
1	-2.250594	2.666737	0.859483	-2.059458	2.778252	0.338583
1	-2.692527	1.744497	-1.283628	-2.528966	1.539212	-1.667585
1	-1.221184	0.304827	-2.521545	-1.091494	-0.229874	-2.538778
1	-0.169121	3.380531	1.693503	0.041146	3.707662	0.899889
1	1.998712	2.719682	1.031368	2.221497	2.851926	0.416879
6	1.374311	-0.438674	-2.077480	1.449744	-0.992775	-1.797507
1	0.990224	-1.109690	-2.839066	1.033337	-1.818621	-2.381666
6	2.687401	-0.445056	-1.538414	2.730723	-0.976217	-1.156207
1	3.488818	-1.117209	-1.828139	3.480201	-1.771250	-1.201856
6	2.762783	0.563269	-0.535913	2.844979	0.252336	-0.431583
1	3.633367	0.822812	0.057121	3.696546	0.578187	0.172126
25	-1.368112	-0.115091	0.287384	-1.293158	-0.017546	0.252434
6	-3.076541	-0.655061	-0.005075	-2.987613	-0.519757	-0.043035
6	-0.623605	-1.787645	0.235144	-0.711645	-1.717097	0.458577
8	-4.161422	-1.032096	-0.209818	-4.086225	-0.904424	-0.254391
8	0.058300	-2.766549	0.095120	-0.111390	-2.770537	0.544347
25	1.227692	-0.841942	0.095690	1.131723	-0.815623	0.343505
6	1.264621	-0.604916	1.889735	0.841262	-0.051973	1.946840
8	1.335112	-0.383114	3.035156	0.671900	0.508383	2.979892

3T-8

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.066016	-2.137490	0.627686	-1.119406	-2.171559	0.652902
6	-1.064118	-1.227169	1.727450	-1.105360	-1.250971	1.751115
6	-0.547698	0.086241	1.767881	-0.532949	0.052776	1.797153
6	-0.705163	-1.925863	-0.735535	-0.737300	-1.973838	-0.712236
6	0.418303	0.629580	0.823087	0.419675	0.593153	0.844538
6	-0.100258	-0.786875	-1.309445	-0.078207	-0.851086	-1.289893
6	0.632222	0.222474	-0.561735	0.636237	0.169554	-0.553330
1	-1.691941	-3.014655	0.785570	-1.787613	-3.029609	0.804748
1	-1.662045	-1.540649	2.582093	-1.727479	-1.539523	2.608028
1	-0.718283	0.672676	2.668329	-0.708895	0.653811	2.697854
1	-1.077536	-2.678940	-1.428519	-1.130475	-2.719663	-1.414773
1	0.025016	-0.767571	-2.389801	0.048527	-0.841114	-2.379190
6	1.195883	1.818786	1.035885	1.188294	1.804110	1.041848
1	1.232503	2.368046	1.971804	1.228800	2.357559	1.985206
6	1.824150	2.193467	-0.184979	1.822886	2.174860	-0.184883
1	2.468369	3.055795	-0.328522	2.458453	3.052388	-0.337321
6	1.515338	1.208176	-1.162838	1.530935	1.160660	-1.161896
1	1.805850	1.209906	-2.207514	1.816447	1.158153	-2.216879
25	-1.666886	-0.127966	-0.025717	-1.630782	-0.137256	-0.013377
6	-2.155024	1.530277	-0.538925	-2.130149	1.511051	-0.496472
6	-3.401679	-0.522464	-0.184109	-3.359105	-0.452429	-0.219216
8	-4.544628	-0.726884	-0.302519	-4.524637	-0.593604	-0.374334
8	-2.547004	2.576731	-0.873048	-2.556020	2.566576	-0.818250
25	2.658617	0.242927	0.415756	2.630279	0.267369	0.389299
6	3.464598	-1.157999	-0.379070	3.445534	-1.103645	-0.413103
8	3.936826	-2.070536	-0.944001	3.946693	-2.013050	-0.993029

2T-1

	B3LYP			BP86		
	x	y	z	x	y	z
6	-2.668643	-0.308889	1.182857	-2.651691	-0.342012	1.185898
6	-1.450795	-0.044341	1.879823	-1.407945	-0.094827	1.867021
6	-0.130539	-0.607140	1.721462	-0.099729	-0.704132	1.713129
6	-2.782792	-0.783827	-0.149251	-2.788203	-0.789011	-0.159708
6	0.276208	-1.530456	0.694585	0.296593	-1.589411	0.643191
6	-1.667938	-0.997963	-1.012319	-1.660407	-0.957098	-1.046247
6	-0.313425	-1.412593	-0.645505	-0.306820	-1.399888	-0.695578
1	-3.584848	0.052613	1.650879	-3.564418	0.028188	1.675206
1	-1.570374	0.571624	2.773363	-1.506953	0.528976	2.769057
1	0.535118	-0.495074	2.576539	0.575219	-0.627156	2.576759
1	-3.773353	-0.761545	-0.602871	-3.789555	-0.750260	-0.608973
1	-1.895393	-1.069603	-2.077858	-1.894207	-0.982405	-2.122491
6	1.688653	-1.799080	0.522108	1.727184	-1.809418	0.449834
1	2.402605	-1.929718	1.327426	2.451822	-1.967346	1.252092
6	1.987123	-1.751389	-0.873340	2.024368	-1.646675	-0.946372
1	2.964532	-1.888419	-1.322092	3.013513	-1.714811	-1.405051
6	0.779207	-1.496842	-1.577787	0.799545	-1.373562	-1.635852
1	0.687112	-1.388527	-2.653837	0.702060	-1.183389	-2.708403
25	-1.453013	0.906382	-0.082408	-1.448565	0.860320	-0.076467
6	2.438975	1.068612	0.571806	2.429627	1.054018	0.561783
8	3.343462	1.660270	1.011490	3.361373	1.650246	0.982264
25	1.070430	0.117143	-0.113942	1.047492	0.115628	-0.083702
6	0.324526	1.442018	-1.025953	0.252137	1.477569	-0.924951
8	-0.478988	2.171213	-1.573207	-0.567447	2.264274	-1.419371

2S-2

	B3LYP			BP86		
	x	y	z	x	y	z
6	-2.707235	-0.761957	-0.897892	-2.516114	-0.862361	-0.977925
6	-2.771686	-0.462490	0.487560	-2.595843	-0.733428	0.441951
6	-1.648355	-0.383394	1.353845	-1.451232	-0.653094	1.307710
6	-1.572657	-1.091312	-1.696816	-1.351309	-1.011779	-1.787692
6	-0.334101	-0.982548	1.168533	-0.127854	-1.287749	1.150378
6	-0.253225	-1.473968	-1.317486	-0.008084	-1.401660	-1.389469
6	0.224952	-1.739622	0.024926	0.453979	-1.861293	-0.082583
1	-3.609689	-0.528543	-1.463106	-3.440689	-0.624381	-1.524007
1	-3.721578	-0.089594	0.866048	-3.572968	-0.461438	0.862038
1	-1.816885	0.066839	2.332109	-1.650077	-0.284908	2.324665
1	-1.738594	-1.021341	-2.771392	-1.491920	-0.854582	-2.864629
1	0.413830	-1.755722	-2.130610	0.682008	-1.584489	-2.223320
6	0.803457	-0.649162	2.006624	0.988654	-0.860767	1.972033
1	0.747527	-0.056668	2.914466	0.892853	-0.333097	2.925689
6	1.970995	-1.261013	1.483167	2.216963	-1.222448	1.333959
1	2.962111	-1.198000	1.918818	3.217868	-1.023810	1.725428
6	1.633157	-1.933900	0.271132	1.909759	-1.839250	0.086452
1	2.320132	-2.445344	-0.393452	2.626383	-2.173750	-0.668183
25	-1.137389	0.668141	-0.359797	-1.128843	0.660563	-0.280358
6	-0.587266	2.202628	0.342496	-0.690714	2.107234	0.658024
8	-0.349368	3.277941	0.751727	-0.543347	3.110457	1.280361
25	1.012544	0.081230	-0.008631	0.871565	0.078498	-0.022227
6	2.453477	0.727628	-0.912624	1.927799	1.166684	-1.007037
8	3.386267	1.115654	-1.494596	2.622405	1.842467	-1.683843

2T-3

	B3LYP			BP86		
	x	y	z	x	y	z
6	-1.081081	-2.261763	0.591133	-1.234659	-2.275366	0.598946
6	-1.217235	-1.329484	1.666454	-1.351446	-1.329299	1.672813
6	-0.941170	0.064673	1.638454	-0.991111	0.059774	1.655450
6	-0.767688	-1.985293	-0.775087	-0.856785	-2.030156	-0.763638
6	0.043073	0.713268	0.761985	0.029495	0.669829	0.797140
6	-0.356983	-0.744280	-1.330597	-0.357627	-0.804268	-1.311301
6	0.317003	0.329024	-0.602002	0.350652	0.237436	-0.565879
1	-1.474577	-3.259053	0.787340	-1.739314	-3.235789	0.775339
1	-1.739775	-1.707395	2.546187	-1.943447	-1.669396	2.534506
1	-1.244277	0.636834	2.514291	-1.303694	0.655393	2.523743
1	-0.990896	-2.787551	-1.478851	-1.124700	-2.819540	-1.479591
1	-0.278090	-0.703027	-2.416083	-0.252749	-0.765836	-2.403769
6	0.764154	1.921609	1.028207	0.762795	1.884456	1.059452
1	0.742833	2.470231	1.965102	0.729381	2.447691	1.997269
6	1.455430	2.310087	-0.161178	1.529765	2.221993	-0.109775
1	2.088660	3.185111	-0.271896	2.205868	3.076334	-0.211228
6	1.207124	1.324349	-1.160998	1.293793	1.213212	-1.107467
1	1.565713	1.335055	-2.184533	1.705740	1.189927	-2.119682
25	-2.178027	-0.532046	-0.073284	-2.085662	-0.434226	-0.102803
6	-2.971728	1.032172	-0.632643	-2.806130	1.121278	-0.718565
8	-3.469057	2.030512	-0.981268	-3.317963	2.112333	-1.114881
25	2.252205	0.376542	0.480791	2.154501	0.296312	0.550670
6	3.161177	-0.930027	-0.360127	3.119647	-0.867165	-0.385309
8	3.694493	-1.774091	-0.972585	3.701914	-1.617494	-1.103176

2S-4

	B3LYP			BP86		
	x	y	z	x	y	z
6	1.273787	2.343556	0.548172	1.286635	2.351188	0.508850
6	1.342478	1.452436	1.666173	1.315841	1.489278	1.661591
6	0.894192	0.108796	1.751030	0.836740	0.145732	1.789483
6	0.842332	2.117290	-0.798104	0.862619	2.109746	-0.843561
6	-0.001744	-0.546620	0.815023	0.012029	-0.558527	0.831284
6	0.259013	0.947798	-1.345098	0.259961	0.927261	-1.379580
6	-0.303309	-0.150065	-0.585148	-0.313774	-0.158763	-0.616125
1	1.872909	3.245080	0.670834	1.906756	3.250475	0.622479
1	1.944659	1.811908	2.499929	1.921958	1.862459	2.497666
1	1.141176	-0.448957	2.653343	1.088636	-0.395047	2.712333
1	1.132301	2.890874	-1.507965	1.184298	2.865531	-1.572076
1	0.090029	0.924123	-2.420557	0.143474	0.869601	-2.470499
6	-0.594292	-1.852560	1.022337	-0.587013	-1.875290	1.033406
1	-0.504750	-2.432631	1.934804	-0.522708	-2.445932	1.964549
6	-1.245663	-2.250074	-0.180776	-1.268380	-2.269631	-0.163885
1	-1.812670	-3.166831	-0.319210	-1.847579	-3.190537	-0.291013
6	-1.097901	-1.228158	-1.153243	-1.119928	-1.247458	-1.158245
1	-1.468431	-1.246580	-2.171889	-1.513393	-1.272748	-2.177709
25	1.815538	0.327158	-0.105029	1.749319	0.301442	-0.084399
6	2.689852	-1.117415	-0.670722	2.601872	-1.113359	-0.661555
8	3.376033	-1.993129	-1.044163	3.304587	-1.997410	-1.049315
25	-2.115621	-0.440593	0.539599	-2.032796	-0.437144	0.516000
6	-3.020517	0.839008	-0.344596	-2.921066	0.874733	-0.319166
8	-3.516348	1.652493	-1.025066	-3.438053	1.722323	-0.972027

Complete Gaussian Reference

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