Electronic Supplementary Material (ESI) for Chemical Science.

Calculated coordinates, energies and vibrational frequencies for the computational chemistry in:

A comprehensive understanding of carbon-carbon bond formation through alkyne migratory insertion into manganacycles.

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2aa

SCF Energy (au) BP86/SV(P)	-2427.867667755
SCF Energy (au) PBE0/def2-TZVPP	-2427.429781153
SCF Energy (au) PBE0/def2-TZVPP	-2427.4405898830 (Toluene Correction)
Zero Point Energy (au)	0.2962891
Chemical Potential (kJ mol^{-1})	622.29
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06324694

xyz coordinates
43

Mn	1.4645116	0.2343712	0.5909323
C	1.7816619	0.4425193	2.3507023
C	3.1502517	-0.3752202	0.3332030
C	1.9986404	1.9297007	0.2215559
O	2.3604200	3.0246807	0.0388304
O	4.2519496	-0.6744970	0.1185508
O	1.9860597	0.5565279	3.4908732
C	-1.3688135	-0.1875101	1.3527343
C	-1.0731050	1.9759850	0.4993644
C	-2.4254157	2.2929513	0.6800968
C	-3.2774363	1.3187041	1.2262739
C	-2.7416292	0.0711722	1.5626743
C	-0.6964351	-1.4521885	1.6603519
C	0.6639318	-1.4851738	1.3612258
C	1.4083399	-2.7154182	1.6139593
O	0.6707753	-3.7894906	2.2061021
C	-0.6513101	-3.7241982	2.4956329
C	-1.3727373	-2.5906643	2.2321973
H	-0.3769659	2.7177069	0.0793093
H	-2.7928098	3.2910274	0.3962989
H	-4.3469456	1.5296005	1.3888023
H	-3.3841721	-0.7119417	1.9907119
O	2.5769801	-2.9477696	1.3720105
C	-1.1727391	-4.9896275	3.1068736
H	-2.4446006	-2.5726096	2.4751610
N	-0.5455730	0.7755408	0.8231995
C	0.8586201	1.2727425	-2.6141879
C	1.9732273	2.0182441	-3.0776447
C	1.8089943	2.9990900	-4.0649810
C	0.5359603	3.2632459	-4.6022414
C	-0.5765511	2.5332325	-4.1481913
C	-0.4219365	1.5470344	-3.1628167
H	2.9715633	1.8130324	-2.6613145
H	2.6864145	3.5651591	-4.4186222
H	0.4115198	4.0380631	-5.3765206
H	-1.5768983	2.7310968	-4.5679957
H	-1.2907383	0.9686119	-2.8108704
C	1.0036831	0.2255046	-1.6318907
C	0.9714273	-0.9282526	-1.1151016
H	0.8955204	-2.0110916	-1.2178750
H	-1.0093753	-5.8521617	2.4222750
H	-2.2559519	-4.9078343	3.3298297
H	-0.6283127	-5.2198957	4.0505213

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-

6		0.00	0.00000	-	-
7	a	12.83	0.33682	YES	YES
8	a	28.85	0.53951	YES	YES
9	a	32.31	0.18001	YES	YES
10	a	37.53	1.95531	YES	YES
11	a	60.15	0.05712	YES	YES
12	a	69.85	0.11556	YES	YES
13	a	75.55	0.07607	YES	YES
14	a	81.69	0.39008	YES	YES
15	a	91.73	1.64917	YES	YES
16	a	99.05	0.97666	YES	YES
17	a	109.88	0.12991	YES	YES
18	a	119.87	0.10005	YES	YES
19	a	123.49	1.49253	YES	YES
20	a	137.69	0.14153	YES	YES
21	a	148.69	1.92865	YES	YES
22	a	153.79	1.84421	YES	YES
23	a	159.65	1.34880	YES	YES
24	a	163.44	2.66553	YES	YES
25	a	192.46	1.04417	YES	YES
26	a	219.28	0.63073	YES	YES
27	a	249.36	0.36492	YES	YES
28	a	257.61	1.89803	YES	YES
29	a	294.76	2.37808	YES	YES
30	a	302.79	4.27708	YES	YES
31	a	322.17	10.76010	YES	YES
32	a	330.22	13.32318	YES	YES
33	a	398.32	4.09474	YES	YES
34	a	401.54	0.07874	YES	YES
35	a	414.56	12.49803	YES	YES
36	a	428.96	1.22830	YES	YES
37	a	455.65	0.76864	YES	YES
38	a	457.06	9.03126	YES	YES
39	a	467.19	5.31735	YES	YES
40	a	479.14	10.45341	YES	YES
41	a	486.43	4.00283	YES	YES
42	a	493.29	15.20698	YES	YES
43	a	500.80	11.90031	YES	YES
44	a	521.26	39.87505	YES	YES
45	a	532.31	6.17382	YES	YES
46	a	537.42	1.03599	YES	YES
47	a	544.56	5.83322	YES	YES
48	a	561.68	1.89963	YES	YES
49	a	581.56	3.53684	YES	YES
50	a	590.09	1.38142	YES	YES

2aa'

SCF Energy (au) BP86/SV(P) -2427.867511092
SCF Energy (au) PBE0/def2-TZVPP -2427.429306722
SCF Energy (au) PBE0/def2-TZVPP -2427.4398029146 (Toluene Correction)
Zero Point Energy (au) 0.2965857
Chemical Potential (kJ mol^{-1}) 627.02
Dispersion Correction (au) PBE0/def2-TZVPP -0.06502154

xyz coordinates
43

Mn	1.5147523	1.8031815	0.1393490
C	1.7127939	2.1387468	1.9018085
C	3.2493306	1.2886291	-0.0008400
C	1.9281023	3.5153518	-0.2748048
O	2.1937308	4.6255178	-0.5219659
O	4.3733880	1.0453489	-0.1588772
O	1.8492529	2.3558813	3.0367268
C	-1.3079859	1.1705764	0.7982681
C	-1.1705494	3.2587826	-0.2561876
C	-2.5571983	3.4451580	-0.1964264
C	-3.3444393	2.4413384	0.3921436
C	-2.7119508	1.2979551	0.8908193
C	-0.5340596	0.0226442	1.2788665
C	0.8392402	0.0971972	1.0533379
C	1.6869353	-0.9837612	1.5445888
O	1.0171909	-2.0733219	2.1814486
C	-0.3230854	-2.1275936	2.3677577
C	-1.1327676	-1.1103397	1.9381859
H	-0.5218856	4.0264367	-0.7056722
H	-3.0024165	4.3659229	-0.6039621
H	-4.4391991	2.5486993	0.4604218
H	-3.3026868	0.4929847	1.3514589
O	2.8988123	-1.0795146	1.4755477
C	-0.7602480	-3.3773999	3.0697511
H	-2.2161667	-1.1829428	2.1088455
N	-0.5509876	2.1614445	0.2266401
H	1.5437899	2.6770580	-2.7278962
C	1.3490132	1.8945099	-1.9927118
C	1.1035637	0.6840225	-1.6983683
C	0.7228759	-0.6759224	-2.0148629
H	-0.4580107	-4.2776405	2.4886854
H	-1.8604484	-3.3925945	3.2075539
H	-0.2712121	-3.4569603	4.0667827
C	-0.0173112	-3.3078536	-2.7473764
C	-0.8258252	-2.2191517	-3.1181057
C	-0.4617625	-0.9130270	-2.7582148
C	1.5263381	-1.7809469	-1.6370200
C	1.1589866	-3.0817693	-2.0096625
H	-0.3036529	-4.3333910	-3.0337641
H	-1.7490587	-2.3869893	-3.6976299
H	-1.0910542	-0.0579195	-3.0525480
H	2.4456298	-1.6090748	-1.0558656
H	1.8002357	-3.9292733	-1.7162254

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-

6		0.00	0.00000	-	-
7	a	24.31	0.19772	YES	YES
8	a	26.79	0.77570	YES	YES
9	a	44.61	0.64194	YES	YES
10	a	50.58	0.51026	YES	YES
11	a	66.00	0.33144	YES	YES
12	a	72.98	0.69452	YES	YES
13	a	77.43	0.43971	YES	YES
14	a	83.41	0.66789	YES	YES
15	a	95.16	0.95452	YES	YES
16	a	100.70	0.38104	YES	YES
17	a	106.25	0.32277	YES	YES
18	a	124.35	0.25320	YES	YES
19	a	127.92	0.85768	YES	YES
20	a	138.50	0.05127	YES	YES
21	a	150.94	0.32827	YES	YES
22	a	158.78	1.28351	YES	YES
23	a	166.59	0.35274	YES	YES
24	a	180.24	1.66707	YES	YES
25	a	188.29	2.27493	YES	YES
26	a	212.55	0.37909	YES	YES
27	a	247.14	0.72321	YES	YES
28	a	260.96	0.15337	YES	YES
29	a	294.50	3.08395	YES	YES
30	a	308.25	8.36217	YES	YES
31	a	326.79	2.69630	YES	YES
32	a	337.65	8.35710	YES	YES
33	a	398.14	3.36635	YES	YES
34	a	403.18	2.34038	YES	YES
35	a	408.53	10.62109	YES	YES
36	a	428.45	10.50586	YES	YES
37	a	457.68	0.58035	YES	YES
38	a	460.91	0.98099	YES	YES
39	a	468.88	4.53489	YES	YES
40	a	479.50	3.90853	YES	YES
41	a	484.74	7.08867	YES	YES
42	a	493.18	4.58799	YES	YES
43	a	506.36	23.83062	YES	YES
44	a	525.23	14.38684	YES	YES
45	a	535.01	3.26780	YES	YES
46	a	541.18	0.57910	YES	YES
47	a	559.77	3.82363	YES	YES
48	a	564.37	1.56700	YES	YES
49	a	583.10	1.77315	YES	YES
50	a	593.14	1.93748	YES	YES

2ba

SCF Energy (au)BP86/SV(P) -2277.516190056
SCF Energy (au)PBE0/def2-TZVPP -2277.070640511
SCF Energy (au)PBE0/def2-TZVPP -2277.0778650907 (Toluene Correction)
Zero Point Energy (au) 0.2897773
Chemical Potential (kJ mol^{-1}) 615.66
Dispersion Correction (au) PBE0/def2-TZVPP -0.06110662

xyz coordinates
41

Mn	1.3218603	0.2161020	0.6121444
C	1.7788652	0.6991612	2.2861199
C	3.0068573	-0.2730204	0.2487755
C	1.5913757	1.8997864	-0.0160227
O	1.8059907	2.9928522	-0.3644069
O	4.1007668	-0.6058230	0.0151684
O	2.0820196	1.0031429	3.3682155
C	-1.3180498	-0.4492854	1.7886866
C	-1.4278286	1.5987142	0.6433287
C	-2.7843206	1.7644718	0.9428058
C	-3.4261769	0.7711469	1.7027561
C	-2.6879074	-0.3376577	2.1237114
C	-0.4446517	-1.5624103	2.1751019
C	0.9072958	-1.4767290	1.7297269
C	1.7860999	-2.5181232	2.0955425
C	1.3438020	-3.6150948	2.8558307
C	0.0029626	-3.6950653	3.2795373
C	-0.8868254	-2.6697164	2.9404323
H	-0.8883399	2.3555919	0.0531607
H	-3.3179336	2.6588013	0.5861152
H	-4.4929401	0.8621691	1.9652861
H	-3.1679721	-1.1282940	2.7185786
H	2.8433831	-2.4844404	1.7833064
H	2.0545812	-4.4155643	3.1237603
H	-0.3442870	-4.5537096	3.8769362
H	-1.9343081	-2.7352412	3.2784777
N	-0.7068340	0.5308017	1.0490580
C	0.4186177	0.7604854	-2.6526220
C	1.4639894	1.4883082	-3.2758567
C	1.2035674	2.2810818	-4.4019640
C	-0.1001745	2.3746674	-4.9216796
C	-1.1459588	1.6622080	-4.3088994
C	-0.8936096	0.8615517	-3.1851924
H	2.4862082	1.4183505	-2.8726273
H	2.0294261	2.8347075	-4.8783822
H	-0.3004026	3.0034950	-5.8047658
H	-2.1704367	1.7271619	-4.7118877
H	-1.7103084	0.2966645	-2.7081434
C	0.6611091	-0.1065099	-1.5221846
C	0.6813710	-1.1757627	-0.8449443
H	0.5791166	-2.2589761	-0.7729843

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.14	0.20009	YES	YES

8	a	29.04	0.15401	YES	YES
9	a	39.82	0.05836	YES	YES
10	a	57.15	0.31155	YES	YES
11	a	69.46	0.07269	YES	YES
12	a	74.18	0.09666	YES	YES
13	a	86.23	1.28775	YES	YES
14	a	90.54	0.26084	YES	YES
15	a	99.10	0.43721	YES	YES
16	a	109.57	0.13096	YES	YES
17	a	113.25	0.10437	YES	YES
18	a	117.38	0.59846	YES	YES
19	a	130.55	0.29161	YES	YES
20	a	162.17	1.81464	YES	YES
21	a	165.28	5.13092	YES	YES
22	a	188.98	1.29120	YES	YES
23	a	222.35	0.64998	YES	YES
24	a	242.82	2.12591	YES	YES
25	a	262.80	0.48548	YES	YES
26	a	282.79	1.96336	YES	YES
27	a	319.03	24.25280	YES	YES
28	a	358.43	1.93112	YES	YES
29	a	400.88	0.01385	YES	YES
30	a	410.80	1.69648	YES	YES
31	a	420.57	10.80509	YES	YES
32	a	437.44	2.27242	YES	YES
33	a	454.64	16.81944	YES	YES
34	a	456.28	1.42207	YES	YES
35	a	472.05	4.20216	YES	YES
36	a	480.46	6.23593	YES	YES
37	a	486.64	1.87109	YES	YES
38	a	492.13	5.61083	YES	YES
39	a	502.05	7.64352	YES	YES
40	a	508.50	13.02943	YES	YES
41	a	524.55	36.11294	YES	YES
42	a	539.45	10.10604	YES	YES
43	a	551.07	5.77890	YES	YES
44	a	557.04	1.74908	YES	YES
45	a	609.09	21.17504	YES	YES
46	a	614.47	7.83987	YES	YES
47	a	623.39	7.80591	YES	YES
48	a	625.85	11.54609	YES	YES
49	a	643.05	9.93463	YES	YES
50	a	653.95	72.74795	YES	YES

2ba'

SCF Energy (au) BP86/SV(P) -2277.513915506
SCF Energy (au)PBE0/def2-TZVPP -2277.068149867
SCF Energy (au) PBE0/def2-TZVPP -2277.0753739100 (Toluene Correction)
Zero Point Energy (au) 0.2897742
Chemical Potential (kJ mol^{-1}) 615.97
Dispersion Correction (au) PBE0/def2-TZVPP -0.06339944

xyz coordinates
41

Mn	1.2258585	1.7959458	0.2361359
C	1.3726238	2.2084123	1.9870298
C	2.9819188	1.4607606	0.1062994
C	1.4143764	3.5362389	-0.2348193
O	1.5584791	4.6599386	-0.5184893
O	4.1193272	1.2134699	0.0247307
O	1.4762395	2.4873278	3.1120387
C	-1.4586829	0.7709355	0.9713587
C	-1.6429054	2.8509145	-0.1047515
C	-3.0388337	2.8435896	-0.0183476
C	-3.6627762	1.7421360	0.5941326
C	-2.8677031	0.7049515	1.0873249
C	-0.5234072	-0.2504435	1.4522467
C	0.8585732	0.0090274	1.2153396
C	1.7918361	-0.9298249	1.7020787
C	1.3783681	-2.0989935	2.3648978
C	0.0097808	-2.3548680	2.5709695
C	-0.9371225	-1.4300543	2.1171572
H	-1.1144621	3.6948098	-0.5748638
H	-3.6178365	3.6883408	-0.4221460
H	-4.7602400	1.6941301	0.6854248
H	-3.3329288	-0.1690477	1.5661469
H	2.8730423	-0.7571295	1.5689616
H	2.1337988	-2.8169591	2.7274855
H	-0.3163077	-3.2707270	3.0901531
H	-2.0076893	-1.6308725	2.2885396
N	-0.8676015	1.8541483	0.3737200
H	1.0761801	2.5805694	-2.6558619
C	0.9964970	1.8046790	-1.8925299
C	0.8866792	0.5828388	-1.5683411
C	0.6452584	-0.8197349	-1.8227326
C	0.1610902	-3.5448254	-2.4166148
C	1.4167314	-3.1382082	-1.9305350
C	1.6585020	-1.7912392	-1.6274982
C	-0.6176938	-1.2392218	-2.3130126
C	-0.8537739	-2.5906422	-2.6051716
H	-0.0258660	-4.6064105	-2.6487203
H	2.2185010	-3.8805090	-1.7827013
H	2.6422624	-1.4735862	-1.2495178
H	-1.4095959	-0.4891813	-2.4676116
H	-1.8404977	-2.9006858	-2.9879057

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.53	0.21377	YES	YES

8	a	27.79	0.28921	YES	YES
9	a	45.99	0.13612	YES	YES
10	a	51.80	0.05357	YES	YES
11	a	64.59	0.06234	YES	YES
12	a	74.37	0.68844	YES	YES
13	a	87.29	0.50886	YES	YES
14	a	95.39	0.82393	YES	YES
15	a	97.32	0.37309	YES	YES
16	a	105.55	0.26004	YES	YES
17	a	113.04	0.17732	YES	YES
18	a	118.41	0.31008	YES	YES
19	a	133.64	0.12211	YES	YES
20	a	171.70	2.18610	YES	YES
21	a	174.78	1.43021	YES	YES
22	a	190.88	0.74865	YES	YES
23	a	218.04	0.51180	YES	YES
24	a	233.98	1.36411	YES	YES
25	a	264.26	0.52714	YES	YES
26	a	284.82	0.40484	YES	YES
27	a	325.68	12.47841	YES	YES
28	a	358.71	2.00023	YES	YES
29	a	399.66	1.03863	YES	YES
30	a	405.23	14.09467	YES	YES
31	a	418.07	2.17454	YES	YES
32	a	435.09	3.43305	YES	YES
33	a	457.07	1.70795	YES	YES
34	a	461.68	1.61109	YES	YES
35	a	469.82	4.73183	YES	YES
36	a	483.44	7.46993	YES	YES
37	a	488.14	0.26797	YES	YES
38	a	493.44	2.16853	YES	YES
39	a	502.03	3.50546	YES	YES
40	a	504.26	20.34088	YES	YES
41	a	528.28	12.34652	YES	YES
42	a	537.56	7.68174	YES	YES
43	a	556.97	2.32393	YES	YES
44	a	567.16	3.05453	YES	YES
45	a	612.23	15.52465	YES	YES
46	a	614.71	25.81800	YES	YES
47	a	623.17	8.97027	YES	YES
48	a	626.79	23.25932	YES	YES
49	a	642.59	20.75191	YES	YES
50	a	649.69	29.46792	YES	YES

2bb

SCF Energy (au) BP86/SV(P) -2505.237954427
SCF Energy (au) PBE0/def2-TZVPP -2504.790885075
SCF Energy (au) PBE0/def2-TZVPP -2504.7995679455 (Toluene Correction)
Zero Point Energy (au) 0.3320389
Chemical Potential (kJ mol^{-1}) 708.87
Dispersion Correction (au) PBE0/def2-TZVPP -0.06626996

xyz coordinates
47

Mn	1.6180000	0.5959888	1.9890749
C	1.6037650	1.0178592	3.7432338
C	3.3429124	0.1140385	2.0743823
C	2.0168363	2.3041750	1.5309996
O	2.2898686	3.4104105	1.2738312
O	4.4599601	-0.2173966	2.1300973
O	1.6041205	1.2900572	4.8745535
C	-1.2314929	-0.1224433	2.4276854
C	-1.0754915	1.9328046	1.3034667
C	-2.4658745	2.0706299	1.2336300
C	-3.2650505	1.0631172	1.7984665
C	-2.6424082	-0.0364777	2.3952798
C	-0.4700380	-1.2378566	3.0025114
C	0.9489658	-1.1392561	2.9070916
C	1.7198929	-2.1869073	3.4518553
C	1.1128659	-3.3042942	4.0519685
C	-0.2897640	-3.3964114	4.1319232
C	-1.0772339	-2.3642047	3.6093205
H	-0.4188630	2.7004377	0.8690315
H	-2.9019077	2.9514510	0.7386382
H	-4.3648766	1.1315375	1.7692289
H	-3.2468539	-0.8421105	2.8369312
H	2.8210083	-2.1434225	3.4119037
H	1.7424419	-4.1107013	4.4656753
H	-0.7662818	-4.2702563	4.6055253
H	-2.1750040	-2.4390751	3.6791968
N	-0.4669697	0.8778050	1.8856129
C	1.9148815	1.3242364	-1.3107508
C	1.6162769	0.4110700	-0.1848834
C	1.3516612	-0.7098415	0.3370742
H	1.1006053	-1.7696478	0.3104107
H	3.0138820	1.3998505	-1.4583892
O	1.4025969	0.8166996	-2.5617656
H	1.5066926	2.3409297	-1.1390848
C	0.1106493	1.1518490	-2.8526820
O	-0.5779918	1.8559542	-2.1311994
C	-0.3415613	0.5661932	-4.1515026
C	-1.2980410	-0.4808569	-6.5823375
C	-2.1297592	0.3353950	-5.7937381
C	-1.6539717	0.8572538	-4.5829244
C	0.4903588	-0.2538503	-4.9450346
C	0.0102220	-0.7740441	-6.1565301
H	-1.6719762	-0.8915143	-7.5350248
H	-3.1552568	0.5653103	-6.1266224
H	-2.2846628	1.4989506	-3.9479393
H	1.5114632	-0.4793423	-4.6037506
H	0.6614034	-1.4140937	-6.7744408

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.78	0.63109	YES	YES
8	a	16.17	0.06385	YES	YES
9	a	26.51	0.94380	YES	YES
10	a	40.83	0.11857	YES	YES
11	a	44.50	0.14099	YES	YES
12	a	60.04	0.64516	YES	YES
13	a	69.03	0.21975	YES	YES
14	a	72.21	0.85703	YES	YES
15	a	84.34	1.45753	YES	YES
16	a	90.90	0.52749	YES	YES
17	a	96.39	0.34389	YES	YES
18	a	97.44	0.34176	YES	YES
19	a	108.60	0.17659	YES	YES
20	a	112.21	0.23145	YES	YES
21	a	134.87	0.21442	YES	YES
22	a	147.43	0.82215	YES	YES
23	a	158.85	0.08209	YES	YES
24	a	184.11	0.56099	YES	YES
25	a	192.44	2.38537	YES	YES
26	a	210.96	1.77207	YES	YES
27	a	233.43	1.65430	YES	YES
28	a	247.96	0.63882	YES	YES
29	a	261.35	0.30126	YES	YES
30	a	284.47	0.09530	YES	YES
31	a	304.39	0.64005	YES	YES
32	a	335.44	25.56220	YES	YES
33	a	352.01	10.82510	YES	YES
34	a	358.09	2.98049	YES	YES
35	a	403.84	0.00135	YES	YES
36	a	404.89	3.35779	YES	YES
37	a	418.21	9.17855	YES	YES
38	a	437.11	1.26946	YES	YES
39	a	443.49	0.54007	YES	YES
40	a	456.37	13.63186	YES	YES
41	a	456.91	1.18641	YES	YES
42	a	470.12	3.60864	YES	YES
43	a	474.64	4.67313	YES	YES
44	a	485.86	2.37910	YES	YES
45	a	492.24	4.47263	YES	YES
46	a	503.55	2.17480	YES	YES
47	a	534.83	27.57216	YES	YES
48	a	551.35	6.93128	YES	YES
49	a	555.83	2.85141	YES	YES
50	a	586.75	24.75587	YES	YES

2bb′

SCF Energy (au) BP86/SV(P)	-2505.236933617
SCF Energy (au) PBE0/def2-TZVPP	-2504.790820918
SCF Energy (au) PBE0/def2-TZVPP	-2504.8004063460 (Toluene Correction)
Zero Point Energy (au)	0.3315667
Chemical Potential (kJ mol^{-1})	706.66
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06608119

xyz coordinates
47

Mn	1.2071453	2.0845764	1.5175484
C	1.5188067	2.4327129	3.2632450
C	2.9535568	1.8067143	1.2210547
C	1.3109007	3.8417076	1.0832671
O	1.3966017	4.9769109	0.8238098
O	4.0859643	1.6046888	1.0311148
O	1.7333257	2.6615735	4.3833466
C	-1.3840104	1.0164804	2.5067439
C	-1.6943190	3.1234148	1.5175162
C	-3.0701762	3.1092395	1.7689236
C	-3.6164244	1.9914272	2.4235040
C	-2.7682459	0.9435312	2.7903655
C	-0.4006485	-0.0225468	2.8330711
C	0.9456160	0.2488490	2.4458893
C	1.9236663	-0.7190291	2.7573426
C	1.5843701	-1.9224081	3.4016184
C	0.2501914	-2.1840534	3.7654303
C	-0.7378730	-1.2338403	3.4845280
H	-1.2264610	3.9816417	1.0106712
H	-3.6935940	3.9614037	1.4575101
H	-4.6949615	1.9379273	2.6444659
H	-3.1737855	0.0566284	3.2988505
H	2.9806457	-0.5440618	2.4946808
H	2.3709950	-2.6637524	3.6227759
H	-0.0168191	-3.1263013	4.2706177
H	-1.7801840	-1.4411310	3.7777907
N	-0.8674528	2.1174004	1.8745210
H	0.7237230	2.9428306	-1.3284374
C	0.7759412	2.1447418	-0.5880217
C	0.7649805	0.9334115	-0.2159492
C	0.6374431	-0.5091082	-0.4762539
H	1.5424555	-1.0611915	-0.1361967
O	0.4464628	-0.7112175	-1.8951661
H	-0.2152662	-0.9533645	0.0840899
C	0.3120342	-2.0094032	-2.2835204
C	0.1420535	-2.1399345	-3.7650974
O	0.3329019	-2.9454306	-1.5003728
C	-0.1749361	-2.5062572	-6.5373558
C	-0.0310494	-1.2097279	-6.0112969
C	0.1273187	-1.0236341	-4.6295330
C	-0.0029913	-3.4390717	-4.2974052
C	-0.1608425	-3.6207548	-5.6784601
H	-0.2979793	-2.6493881	-7.6239929
H	-0.0414565	-0.3366498	-6.6845058
H	0.2423172	-0.0138216	-4.2085190
H	0.0128639	-4.2944664	-3.6037226
H	-0.2728045	-4.6372664	-6.0904863

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.69	0.77150	YES	YES
8	a	14.31	0.44876	YES	YES
9	a	27.98	0.18749	YES	YES
10	a	41.43	0.34307	YES	YES
11	a	51.94	0.21434	YES	YES
12	a	56.54	0.08029	YES	YES
13	a	68.27	0.37237	YES	YES
14	a	70.82	0.45542	YES	YES
15	a	83.57	0.05551	YES	YES
16	a	85.91	0.91697	YES	YES
17	a	96.63	0.69206	YES	YES
18	a	101.41	0.21988	YES	YES
19	a	107.13	0.45072	YES	YES
20	a	111.31	0.30546	YES	YES
21	a	128.18	0.55150	YES	YES
22	a	135.51	0.37011	YES	YES
23	a	157.84	0.40895	YES	YES
24	a	186.62	0.71237	YES	YES
25	a	188.13	0.18813	YES	YES
26	a	206.37	1.05808	YES	YES
27	a	220.77	1.27731	YES	YES
28	a	235.13	0.37823	YES	YES
29	a	265.42	0.69843	YES	YES
30	a	281.00	2.87185	YES	YES
31	a	293.67	13.05060	YES	YES
32	a	322.49	3.95365	YES	YES
33	a	354.65	5.38279	YES	YES
34	a	358.97	1.99179	YES	YES
35	a	396.54	16.64607	YES	YES
36	a	403.91	0.00075	YES	YES
37	a	418.13	3.11457	YES	YES
38	a	436.08	2.26241	YES	YES
39	a	445.18	0.20183	YES	YES
40	a	454.14	2.00641	YES	YES
41	a	458.13	1.36604	YES	YES
42	a	469.31	2.75263	YES	YES
43	a	473.59	6.60098	YES	YES
44	a	487.20	4.16042	YES	YES
45	a	491.46	3.65311	YES	YES
46	a	504.47	3.40863	YES	YES
47	a	529.10	20.02646	YES	YES
48	a	547.18	6.22080	YES	YES
49	a	557.27	2.47483	YES	YES
50	a	585.62	8.21677	YES	YES

2bc

SCF Energy (au) BP86/SV(P)	-2281.120982087
SCF Energy (au) PBE0/def2-TZVPP	-2280.691348894
SCF Energy (au) PBE0/def2-TZVPP	-2280.6975966102 (Toluene Correction)
Zero Point Energy (au)	0.3575200
Chemical Potential (kJ mol^{-1})	791.47
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06509361

xyz coordinates
47

Mn	1.2025069	0.1620360	1.0932740
C	1.9568143	0.6239857	2.6631145
C	2.7626127	-0.4707803	0.4843492
C	1.4816754	1.8042180	0.3880616
O	1.6872442	2.8755222	-0.0350056
O	3.7740952	-0.8988125	0.0895477
O	2.4567165	0.9146208	3.6736798
C	-1.2674439	-0.3023652	2.6745928
C	-1.3912158	1.7610984	1.5612277
C	-2.6659539	2.0309656	2.0698859
C	-3.2584096	1.0819363	2.9213569
C	-2.5540902	-0.0861767	3.2217314
C	-0.4365673	-1.4859299	2.9195833
C	0.8303787	-1.5029309	2.2647405
C	1.6666344	-2.6177159	2.4886735
C	1.2610305	-3.6855246	3.3088101
C	0.0017371	-3.6623661	3.9393346
C	-0.8426867	-2.5634264	3.7452354
H	-0.8890702	2.4838705	0.8994692
H	-3.1751348	2.9700773	1.8036640
H	-4.2600129	1.2541116	3.3483852
H	-2.9958712	-0.8431618	3.8858832
H	2.6605532	-2.6671882	2.0133031
H	1.9364916	-4.5450173	3.4598796
H	-0.3169334	-4.4982914	4.5831522
H	-1.8256840	-2.5481467	4.2443786
N	-0.7037795	0.6342783	1.8461413
C	0.1497651	0.7721964	-2.1486257
C	0.2718754	-0.0683968	-0.9320319
C	0.1891642	-1.1366730	-0.2631221
H	-0.0993771	-2.1746493	-0.1043557
C	1.4730397	0.8028500	-2.9612945
C	-1.0183065	0.2671813	-3.0382063
H	-0.0792297	1.8227280	-1.8535928
C	-1.1565103	1.1132381	-4.3163661
H	-1.9654677	0.2801394	-2.4548417
H	-0.8234627	-0.7970045	-3.3086006
H	2.2961270	1.1998921	-2.3286030
C	1.3263403	1.6449803	-4.2404805
H	1.7477958	-0.2449558	-3.2238571
H	1.1602417	2.7121905	-3.9595975
H	2.2790566	1.6176752	-4.8155415
C	0.1575487	1.1588161	-5.1149762
H	-1.4552353	2.1520586	-4.0381253
H	-1.9808817	0.7083946	-4.9460352
H	0.0445918	1.8137098	-6.0082216
H	0.3872873	0.1367419	-5.4999742

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	21.31	0.24853	YES	YES
8	a	34.94	0.01906	YES	YES
9	a	38.46	0.04270	YES	YES
10	a	56.12	0.16270	YES	YES
11	a	66.63	0.03245	YES	YES
12	a	77.27	0.13836	YES	YES
13	a	83.57	0.79291	YES	YES
14	a	91.64	0.35616	YES	YES
15	a	98.95	0.67833	YES	YES
16	a	107.88	0.25597	YES	YES
17	a	112.19	0.26611	YES	YES
18	a	116.96	0.11094	YES	YES
19	a	125.21	0.31890	YES	YES
20	a	144.42	2.49941	YES	YES
21	a	170.19	2.12557	YES	YES
22	a	188.62	1.02686	YES	YES
23	a	213.81	0.39124	YES	YES
24	a	230.38	0.08836	YES	YES
25	a	242.25	1.38666	YES	YES
26	a	245.53	2.60861	YES	YES
27	a	264.09	0.25243	YES	YES
28	a	284.24	0.01913	YES	YES
29	a	348.77	2.37378	YES	YES
30	a	358.13	2.17632	YES	YES
31	a	381.93	9.42387	YES	YES
32	a	409.55	0.56836	YES	YES
33	a	417.09	5.99506	YES	YES
34	a	425.66	0.41850	YES	YES
35	a	436.05	0.68267	YES	YES
36	a	454.69	13.16624	YES	YES
37	a	457.31	1.49122	YES	YES
38	a	473.52	2.84621	YES	YES
39	a	483.72	3.74094	YES	YES
40	a	493.07	1.51086	YES	YES
41	a	495.13	1.75850	YES	YES
42	a	497.07	5.09040	YES	YES
43	a	505.51	2.43664	YES	YES
44	a	535.73	28.50850	YES	YES
45	a	548.84	10.33325	YES	YES
46	a	557.11	1.46236	YES	YES
47	a	563.44	9.53427	YES	YES
48	a	615.81	12.89888	YES	YES
49	a	624.34	4.08364	YES	YES
50	a	627.92	29.19440	YES	YES

2bc'

SCF Energy (au) BP86/SV(P)	-2281.119860015
SCF Energy (au) PBE0/def2-TZVPP	-2280.690435817
SCF Energy (au) PBE0/def2-TZVPP	-2280.6964385324 (Toluene Correction)
Zero Point Energy (au)	0.3576711
Chemical Potential (kJ mol^{-1})	793.30
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06716635

xyz coordinates

47

Mn	1.0348289	2.0037251	0.7072396
C	1.3546343	2.3648770	2.4445458
C	2.7685807	1.6679846	0.4096337
C	1.1942521	3.7522247	0.2578736
O	1.3200183	4.8827259	-0.0095936
O	3.8951655	1.4302241	0.2189937
O	1.5757112	2.6034661	3.5623050
C	-1.5965905	0.9998528	1.6467973
C	-1.8317482	3.1290658	0.6865140
C	-3.2127062	3.1468550	0.9091137
C	-3.8017169	2.0327022	1.5320069
C	-2.9882074	0.9577381	1.8992821
C	-0.6444245	-0.0631017	1.9870364
C	0.7165889	0.1839616	1.6335863
C	1.6659530	-0.7997902	1.9866181
C	1.2861615	-1.9957063	2.6221302
C	-0.0641999	-2.2359852	2.9407155
C	-1.0246722	-1.2672621	2.6284229
H	-1.3310466	3.9832302	0.2046771
H	-3.8068641	4.0207289	0.6004812
H	-4.8858393	2.0035153	1.7292105
H	-3.4267504	0.0739880	2.3855938
H	2.7350754	-0.6397247	1.7674973
H	2.0539780	-2.7462203	2.8771043
H	-0.3635825	-3.1712938	3.4410703
H	-2.0788268	-1.4523673	2.8937919
N	-1.0386625	2.0959762	1.0422653
H	0.5636553	2.8721143	-2.1221330
C	0.6035118	2.0483260	-1.4099698
C	0.5517948	0.8292798	-1.0716342
C	0.3951208	-0.6125177	-1.3884540
C	1.7673471	-1.2751013	-1.6862411
C	-0.5722618	-0.8124266	-2.5852298
H	-0.0375554	-1.1334973	-0.5047080
C	-0.7282709	-2.3028996	-2.9361699
H	-0.1700283	-0.2584620	-3.4657544
H	-1.5610590	-0.3609318	-2.3471509
H	2.2469902	-0.7321242	-2.5336279
C	1.6047150	-2.7634174	-2.0409011
H	2.4376173	-1.1564950	-0.8086280
H	-1.4020842	-2.4135281	-3.8158544
H	-1.2286084	-2.8281054	-2.0881917
C	0.6309114	-2.9683156	-3.2143939
H	2.5998664	-3.2014382	-2.2815466
H	1.2262434	-3.3119724	-1.1461211
H	0.4947536	-4.0544028	-3.4193741
H	1.0722309	-2.5254750	-4.1388293

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	24.72	0.36389	YES	YES
8	a	41.59	0.07488	YES	YES
9	a	45.25	0.06575	YES	YES
10	a	52.15	0.11210	YES	YES
11	a	63.64	0.04811	YES	YES
12	a	76.29	0.28325	YES	YES
13	a	87.06	0.59299	YES	YES
14	a	94.90	0.57956	YES	YES
15	a	96.08	0.16813	YES	YES
16	a	104.24	0.55311	YES	YES
17	a	111.89	0.16725	YES	YES
18	a	117.23	0.10103	YES	YES
19	a	125.86	0.20698	YES	YES
20	a	155.34	0.95071	YES	YES
21	a	176.64	2.31596	YES	YES
22	a	189.40	0.72962	YES	YES
23	a	217.68	0.38679	YES	YES
24	a	228.82	1.35028	YES	YES
25	a	239.91	0.04320	YES	YES
26	a	252.70	0.27808	YES	YES
27	a	267.89	0.60585	YES	YES
28	a	285.93	0.07364	YES	YES
29	a	357.82	1.81800	YES	YES
30	a	358.68	1.20955	YES	YES
31	a	379.42	12.58201	YES	YES
32	a	413.80	2.47893	YES	YES
33	a	421.06	2.16931	YES	YES
34	a	425.08	1.18950	YES	YES
35	a	436.27	1.59759	YES	YES
36	a	457.23	1.43469	YES	YES
37	a	460.02	1.13592	YES	YES
38	a	472.28	2.42811	YES	YES
39	a	485.41	5.28717	YES	YES
40	a	489.47	2.52597	YES	YES
41	a	494.19	9.12418	YES	YES
42	a	498.54	0.71289	YES	YES
43	a	508.60	2.78867	YES	YES
44	a	529.06	16.45843	YES	YES
45	a	554.23	2.74309	YES	YES
46	a	558.08	2.78602	YES	YES
47	a	580.21	5.14682	YES	YES
48	a	615.69	26.75293	YES	YES
49	a	623.84	7.32930	YES	YES
50	a	627.13	24.83024	YES	YES

2bd

SCF Energy (au) BP86/SV(P)	-2411.386418687
SCF Energy (au) PBE0/def2-TZVPP	-2410.929730749
SCF Energy (au) PBE0/def2-TZVPP	-2410.9384397830 (Toluene Correction)
Zero Point Energy (au)	0.3601077
Chemical Potential (kJ mol^{-1})	781.98
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06936495

xyz coordinates

49

Mn	1.3925957	-0.2876905	1.7876510
C	1.8013007	0.3501230	3.4179483
C	3.0913075	-0.7763907	1.5034861
C	1.6475177	1.3305527	1.0040488
O	1.8535412	2.3906773	0.5573821
O	4.1949478	-1.1118628	1.3195940
O	2.0741051	0.7505419	4.4776491
C	-1.2733784	-0.9329752	2.9018538
C	-1.3729850	1.0364967	1.6250640
C	-2.7435242	1.1929112	1.8591491
C	-3.3985417	0.2359856	2.6539271
C	-2.6578172	-0.8284409	3.1737159
C	-0.3957473	-1.9991732	3.3944334
C	0.9719780	-1.9081982	2.9989035
C	1.8536763	-2.9048410	3.4696009
C	1.4022611	-3.9601422	4.2816231
C	0.0462868	-4.0446748	4.6538200
C	-0.8488814	-3.0647430	4.2109765
H	-0.8228403	1.7657238	1.0107653
H	-3.2774785	2.0527496	1.4261788
H	-4.4767091	0.3212295	2.8676273
H	-3.1472115	-1.5898039	3.7984506
H	2.9227283	-2.8677717	3.1999172
H	2.1173776	-4.7245731	4.6315816
H	-0.3082608	-4.8711275	5.2912563
H	-1.9088144	-3.1333749	4.5079584
N	-0.6495121	0.0106224	2.1251006
C	0.5362402	0.0227771	-1.5621652
C	1.5876226	0.6627500	-2.2691490
C	1.3426892	1.4197705	-3.4145819
C	0.0190698	1.5921664	-3.9213900
C	-1.0380191	0.9549214	-3.2052885
C	-0.7817999	0.1962930	-2.0610430
H	2.6225990	0.5547868	-1.9084296
H	2.1984547	1.8871607	-3.9215151
N	-0.2266218	2.3434817	-5.0577128
H	-2.0784857	1.0466807	-3.5477473
H	-1.6206983	-0.2895092	-1.5372084
C	0.7777766	-0.8031245	-0.4136716
C	0.8486570	-1.7866419	0.3766648
H	0.8017729	-2.8648223	0.5341916
C	-1.5867253	2.5044316	-5.5419388
C	0.8740447	2.9812261	-5.7608789
H	-1.5795323	3.1316451	-6.4551821
H	-2.2440036	3.0052468	-4.7904017
H	-2.0562801	1.5261755	-5.8054631
H	1.4160308	3.7142408	-5.1163019
H	0.4790910	3.5301722	-6.6385994
H	1.6201958	2.2383414	-6.1318513

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.77	0.32390	YES	YES
8	a	19.49	0.47829	YES	YES
9	a	27.15	0.84414	YES	YES
10	a	46.55	0.42645	YES	YES
11	a	59.63	0.00369	YES	YES
12	a	65.68	0.40984	YES	YES
13	a	73.58	0.27310	YES	YES
14	a	77.07	1.07304	YES	YES
15	a	85.22	1.87030	YES	YES
16	a	86.06	0.62738	YES	YES
17	a	93.48	0.56900	YES	YES
18	a	101.53	1.07347	YES	YES
19	a	105.80	0.14299	YES	YES
20	a	110.21	0.77764	YES	YES
21	a	113.50	1.28888	YES	YES
22	a	119.50	10.86627	YES	YES
23	a	145.24	8.95151	YES	YES
24	a	176.05	12.15749	YES	YES
25	a	189.53	2.39487	YES	YES
26	a	211.64	0.15863	YES	YES
27	a	222.89	0.47711	YES	YES
28	a	238.63	2.17760	YES	YES
29	a	247.84	5.48849	YES	YES
30	a	261.30	2.39248	YES	YES
31	a	271.68	15.76820	YES	YES
32	a	287.07	1.13771	YES	YES
33	a	340.00	40.93114	YES	YES
34	a	358.73	1.91607	YES	YES
35	a	380.91	7.35874	YES	YES
36	a	416.00	11.15977	YES	YES
37	a	416.77	1.74031	YES	YES
38	a	430.09	6.89579	YES	YES
39	a	444.10	19.38440	YES	YES
40	a	454.05	5.54465	YES	YES
41	a	456.73	3.22540	YES	YES
42	a	463.11	1.77583	YES	YES
43	a	477.34	6.19032	YES	YES
44	a	488.73	3.79858	YES	YES
45	a	490.92	32.76320	YES	YES
46	a	493.72	5.07364	YES	YES
47	a	503.77	0.62555	YES	YES
48	a	515.82	15.69978	YES	YES
49	a	530.05	43.15597	YES	YES
50	a	541.11	9.60241	YES	YES

2bd'

SCF Energy (au) BP86/SV(P)	-2411.383229723
SCF Energy (au) PBE0/def2-TZVPP	-2410.926493690
SCF Energy (au) PBE0/def2-TZVPP	-2410.9348447962 (Toluene Correction)
Zero Point Energy (au)	0.3602809
Chemical Potential (kJ mol^{-1})	784.73
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07187072

xyz coordinates
49

Mn	1.2663945	2.7708307	0.7416893
C	1.4115506	3.1773508	2.4898686
C	3.0235475	2.4470980	0.6081276
C	1.4377476	4.5142685	0.2781122
O	1.5718707	5.6406263	-0.0035219
O	4.1629481	2.2064819	0.5236885
O	1.5137044	3.4534435	3.6166834
C	-1.4098168	1.6986085	1.4244989
C	-1.6060832	3.7981651	0.3895549
C	-3.0028394	3.7713887	0.4556699
C	-3.6212881	2.6491378	1.0354332
C	-2.8195531	1.6122698	1.5180890
C	-0.4678684	0.6812651	1.8996707
C	0.9129646	0.9617008	1.6764839
C	1.8511667	0.0264272	2.1633669
C	1.4456810	-1.1538910	2.8107245
C	0.0782650	-1.4282234	3.0020761
C	-0.8747426	-0.5094966	2.5486916
H	-1.0820154	4.6583592	-0.0550827
H	-3.5867634	4.6172874	0.0613717
H	-4.7193202	2.5851346	1.1094389
H	-3.2796616	0.7219630	1.9712661
H	2.9317907	0.2123774	2.0422032
H	2.2063352	-1.8663679	3.1738634
H	-0.2418906	-2.3522338	3.5107730
H	-1.9446100	-0.7226850	2.7103168
N	-0.8239537	2.8016353	0.8578603
H	1.1464438	3.5642565	-2.1452500
C	1.0506260	2.7722205	-1.4007081
C	0.9395331	1.5400747	-1.1284499
C	0.6900209	0.1433434	-1.3608377
C	0.1781382	-2.6299613	-1.9369723
C	1.4415419	-2.1922956	-1.4386935
C	1.6820764	-0.8477882	-1.1527721
C	-0.5672552	-0.2881822	-1.8552967
C	-0.8214450	-1.6326957	-2.1363533
N	-0.0659869	-3.9654548	-2.2155184
H	2.2525575	-2.9136067	-1.2664274
H	2.6699657	-0.5470040	-0.7712270
H	-1.3600945	0.4573031	-2.0274221
H	-1.8144344	-1.9063088	-2.5204744
C	-1.3609442	-4.3745029	-2.7290627
C	0.9772797	-4.9540055	-2.0061756
H	-1.6005157	-3.8869288	-3.7054739
H	-2.1894685	-4.1344632	-2.0195169
H	-1.3624895	-5.4706853	-2.8908988
H	1.3071293	-4.9967255	-0.9402114
H	1.8802211	-4.7528585	-2.6321530
H	0.5935398	-5.9566532	-2.2810229

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.44	0.42500	YES	YES
8	a	22.17	0.05493	YES	YES
9	a	36.74	0.87475	YES	YES
10	a	48.62	0.05701	YES	YES
11	a	58.52	1.12493	YES	YES
12	a	66.92	0.69761	YES	YES
13	a	74.69	0.34991	YES	YES
14	a	78.56	0.56269	YES	YES
15	a	84.94	0.59614	YES	YES
16	a	92.36	1.30066	YES	YES
17	a	94.03	0.15738	YES	YES
18	a	97.12	1.58291	YES	YES
19	a	104.13	0.18552	YES	YES
20	a	109.18	0.28495	YES	YES
21	a	117.19	0.83929	YES	YES
22	a	128.57	2.09589	YES	YES
23	a	149.49	6.73147	YES	YES
24	a	184.48	5.05036	YES	YES
25	a	194.26	4.53220	YES	YES
26	a	214.95	0.25485	YES	YES
27	a	216.70	1.13080	YES	YES
28	a	232.49	1.84431	YES	YES
29	a	250.02	1.07986	YES	YES
30	a	263.54	0.20893	YES	YES
31	a	279.47	8.73793	YES	YES
32	a	286.00	0.78289	YES	YES
33	a	338.56	29.90249	YES	YES
34	a	359.12	2.14220	YES	YES
35	a	389.80	11.97136	YES	YES
36	a	414.66	1.31078	YES	YES
37	a	416.05	1.78230	YES	YES
38	a	428.09	10.10769	YES	YES
39	a	441.38	4.97791	YES	YES
40	a	453.54	0.48186	YES	YES
41	a	458.02	1.92772	YES	YES
42	a	467.96	3.93729	YES	YES
43	a	475.17	0.36120	YES	YES
44	a	488.63	5.04201	YES	YES
45	a	491.82	6.89705	YES	YES
46	a	494.74	10.14941	YES	YES
47	a	503.51	1.69264	YES	YES
48	a	515.44	19.65428	YES	YES
49	a	532.86	21.08297	YES	YES
50	a	537.10	6.36060	YES	YES

2be

SCF Energy (au) BP86/SV(P -2391.960168240
SCF Energy (au) PBE0/def2-TZVPP -2391.515765535
SCF Energy (au) PBE0/def2-TZVPP -2391.5241006317 (Toluene Correction)
Zero Point Energy (au) 0.3213065
Chemical Potential (kJ mol^{-1}) 689.58
Dispersion Correction (au) PBE0/def2-TZVPP -0.06471746

xyz coordinates
45

Mn	1.2454519	-0.1636177	1.2461568
C	1.6903274	0.3277975	2.9190853
C	2.9289665	-0.6687297	0.9011828
C	1.5333880	1.5091092	0.6006049
O	1.7617757	2.5966867	0.2410407
O	4.0223501	-1.0121397	0.6782891
O	1.9851445	0.6352659	4.0029599
C	-1.4146805	-0.8122930	2.3802386
C	-1.4917666	1.2371547	1.2347438
C	-2.8522728	1.4111914	1.5105874
C	-3.5136263	0.4212793	2.2581960
C	-2.7895105	-0.6922078	2.6912325
C	-0.5548900	-1.9308340	2.7806847
C	0.8047510	-1.8522571	2.3571412
C	1.6701394	-2.9000083	2.7373162
C	1.2087281	-3.9945510	3.4897093
C	-0.1393528	-4.0664895	3.8914818
C	-1.0169583	-3.0354668	3.5381285
H	-0.9371454	1.9909849	0.6548643
H	-3.3738921	2.3091286	1.1452779
H	-4.5843606	0.5185292	2.5017612
H	-3.2847640	-1.4804512	3.2767930
H	2.7327403	-2.8730782	2.4426186
H	1.9100487	-4.7995708	3.7689854
H	-0.5016334	-4.9231798	4.4828214
H	-2.0703379	-3.0946166	3.8588525
N	-0.7844127	0.1642747	1.6516163
C	0.3793082	0.3930496	-2.0429389
C	1.4345356	1.0980323	-2.6697050
C	1.2055671	1.9129660	-3.7871178
C	-0.1023718	2.0528749	-4.3032530
C	-1.1681430	1.3593666	-3.6828095
C	-0.9317977	0.5456915	-2.5743106
H	2.4585896	0.9989824	-2.2773754
H	2.0563759	2.4375977	-4.2458196
O	-0.4334359	2.8199435	-5.3773085
H	-2.1811248	1.4757238	-4.0991596
H	-1.7678363	0.0040392	-2.1041006
C	0.6035550	-0.4910616	-0.9271151
C	0.6165874	-1.5478216	-0.2322546
H	0.5125044	-2.6303703	-0.1533227
C	0.5904440	3.5378490	-6.0467717
H	0.0933132	4.0802171	-6.8759145
H	1.3640469	2.8545614	-6.4703382
H	1.0856745	4.2764476	-5.3727552

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.73	0.48528	YES	YES
8	a	27.54	0.12557	YES	YES
9	a	33.83	1.31325	YES	YES
10	a	49.40	0.41729	YES	YES
11	a	63.10	0.05113	YES	YES
12	a	68.82	0.12965	YES	YES
13	a	84.84	1.50868	YES	YES
14	a	87.60	0.96268	YES	YES
15	a	94.72	0.65057	YES	YES
16	a	98.26	0.23069	YES	YES
17	a	107.68	0.58782	YES	YES
18	a	111.22	0.26776	YES	YES
19	a	113.72	0.43342	YES	YES
20	a	124.37	0.81217	YES	YES
21	a	142.73	7.98195	YES	YES
22	a	152.38	4.16835	YES	YES
23	a	188.93	1.98886	YES	YES
24	a	208.51	4.11258	YES	YES
25	a	232.84	2.10901	YES	YES
26	a	242.91	6.62047	YES	YES
27	a	251.98	0.82755	YES	YES
28	a	262.32	0.48982	YES	YES
29	a	275.23	8.01602	YES	YES
30	a	286.09	0.47693	YES	YES
31	a	357.60	4.93075	YES	YES
32	a	371.46	41.59569	YES	YES
33	a	401.58	1.57177	YES	YES
34	a	410.70	0.87504	YES	YES
35	a	417.33	7.84680	YES	YES
36	a	431.89	5.36836	YES	YES
37	a	447.02	9.62630	YES	YES
38	a	456.52	1.15156	YES	YES
39	a	461.81	2.74505	YES	YES
40	a	475.05	13.77999	YES	YES
41	a	477.54	10.19568	YES	YES
42	a	488.10	3.35668	YES	YES
43	a	493.60	4.70623	YES	YES
44	a	503.81	2.30819	YES	YES
45	a	521.30	53.32399	YES	YES
46	a	530.71	22.79117	YES	YES
47	a	541.23	7.10764	YES	YES
48	a	551.30	6.72379	YES	YES
49	a	557.16	1.63201	YES	YES
50	a	610.92	29.31754	YES	YES

2be'

SCF Energy (au) BP86/SV(P) -2391.957322776
SCF Energy (au) PBE0/def2-TZVPP -2391.512741707
SCF Energy (au) PBE0/def2-TZVPP -2391.5210557956 (Toluene Correction)
Zero Point Energy (au) 0.3212850
Chemical Potential (kJ mol^{-1}) 689.45
Dispersion Correction (au) PBE0/def2-TZVPP -0.06706478

xyz coordinates
45

Mn	1.2018114	2.3230176	0.7548611
C	1.1966094	2.6674406	2.5251254
C	2.9759053	2.0685991	0.7475998
C	1.3417653	4.0885188	0.3717193
O	1.4525414	5.2294814	0.1461870
O	4.1263842	1.8728426	0.7439207
O	1.2027896	2.9051979	3.6646116
C	-1.4774602	1.1365428	1.2069601
C	-1.6775184	3.2640542	0.2317406
C	-3.0735233	3.1863285	0.1953522
C	-3.6891506	2.0223060	0.6893591
C	-2.8858991	0.9971163	1.1939489
C	-0.5349590	0.1369759	1.7179660
C	0.8469663	0.4745153	1.6144229
C	1.7813724	-0.4410436	2.1429074
C	1.3738901	-1.6595390	2.7139420
C	0.0079458	-1.9916137	2.7849735
C	-0.9429351	-1.0919669	2.2907844
H	-1.1555815	4.1579091	-0.1438556
H	-3.6592854	4.0254717	-0.2104464
H	-4.7864733	1.9171727	0.6805989
H	-3.3436826	0.0755080	1.5820225
H	2.8596110	-0.2102367	2.1153004
H	2.1313858	-2.3568796	3.1110001
H	-0.3134988	-2.9462274	3.2324524
H	-2.0125979	-1.3508374	2.3596834
N	-0.8945810	2.2786934	0.7214380
H	1.2437389	3.2338625	-2.1008219
C	1.1369187	2.4156359	-1.3866901
C	1.0657742	1.1735248	-1.1394614
C	0.9027471	-0.2214474	-1.4706394
C	0.5774429	-2.9415021	-2.2325676
C	1.7520298	-2.5162861	-1.5678323
C	1.9080735	-1.1843100	-1.1866765
C	-0.2675862	-0.6588157	-2.1352765
C	-0.4362164	-1.9999745	-2.5139696
O	0.5206688	-4.2637539	-2.5571430
H	2.5333940	-3.2634943	-1.3587178
H	2.8282443	-0.8669552	-0.6735143
H	-1.0597815	0.0716795	-2.3632990
H	-1.3607870	-2.2966877	-3.0307668
C	-0.6259038	-4.7517284	-3.2312324
H	-0.7672266	-4.2549073	-4.2209286
H	-1.5520862	-4.6194973	-2.6224653
H	-0.4512763	-5.8346902	-3.3925732

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.39	0.19688	YES	YES
8	a	19.98	0.14787	YES	YES
9	a	44.37	0.00775	YES	YES
10	a	48.89	0.01718	YES	YES
11	a	61.20	0.59746	YES	YES
12	a	68.25	0.68447	YES	YES
13	a	81.88	0.18327	YES	YES
14	a	87.08	1.58370	YES	YES
15	a	95.70	0.24980	YES	YES
16	a	97.57	0.86361	YES	YES
17	a	102.60	0.63889	YES	YES
18	a	110.71	0.22605	YES	YES
19	a	117.52	0.87571	YES	YES
20	a	122.30	0.55115	YES	YES
21	a	150.40	5.39288	YES	YES
22	a	161.61	1.44765	YES	YES
23	a	190.00	0.15297	YES	YES
24	a	216.68	1.37135	YES	YES
25	a	225.75	4.27679	YES	YES
26	a	237.39	0.07127	YES	YES
27	a	253.95	0.92664	YES	YES
28	a	264.92	0.43227	YES	YES
29	a	278.53	4.50877	YES	YES
30	a	285.83	0.30984	YES	YES
31	a	358.53	2.62385	YES	YES
32	a	375.40	30.36449	YES	YES
33	a	396.79	5.19120	YES	YES
34	a	411.11	1.55916	YES	YES
35	a	417.35	3.54155	YES	YES
36	a	431.69	7.33705	YES	YES
37	a	441.25	3.09284	YES	YES
38	a	457.69	1.41522	YES	YES
39	a	467.45	2.67182	YES	YES
40	a	473.68	0.88691	YES	YES
41	a	487.20	13.32081	YES	YES
42	a	489.99	5.98088	YES	YES
43	a	492.50	15.77534	YES	YES
44	a	502.67	4.65991	YES	YES
45	a	517.38	1.53708	YES	YES
46	a	531.20	25.42967	YES	YES
47	a	538.74	7.43532	YES	YES
48	a	556.96	2.89561	YES	YES
49	a	566.53	2.71462	YES	YES
50	a	614.64	47.84106	YES	YES

2bf

SCF Energy (au) BP86/SV(P) -2376.686035034
SCF Energy (au) PBE0/def2-TZVPP -2376.263171392
SCF Energy (au) PBE0/def2-TZVPP -2376.2704120363 (Toluene Correction)
Zero Point Energy (au) 0.2818722
Chemical Potential (kJ mol^{-1}) 591.01
Dispersion Correction (au) PBE0/def2-TZVPP -0.06135801

xyz coordinates
41

Mn	1.3698504	0.2105297	0.6366223
C	1.8030365	0.6855900	2.3195994
C	3.0564347	-0.2930315	0.2993493
C	1.6658100	1.8905940	0.0127788
O	1.8958418	2.9812785	-0.3345833
O	4.1506892	-0.6357557	0.0829671
O	2.0890447	0.9837826	3.4077538
C	-1.3001451	-0.4349008	1.7536845
C	-1.3619793	1.6277135	0.6309972
C	-2.7232705	1.8043899	0.9005427
C	-3.3934818	0.8079514	1.6314084
C	-2.6767037	-0.3132861	2.0565742
C	-0.4461613	-1.5590405	2.1509347
C	0.9172178	-1.4817969	1.7399506
C	1.7783799	-2.5325499	2.1201434
C	1.3081757	-3.6313270	2.8607364
C	-0.0437438	-3.7037738	3.2492435
C	-0.9163816	-2.6685955	2.8960569
H	-0.8006641	2.3863890	0.0640316
H	-3.2386840	2.7090901	0.5432493
H	-4.4654821	0.9065288	1.8686038
H	-3.1790790	-1.1058875	2.6299977
H	2.8433144	-2.5053590	1.8343217
H	2.0055263	-4.4394494	3.1405788
H	-0.4129731	-4.5643381	3.8304449
H	-1.9726005	-2.7281497	3.2068953
N	-0.6620770	0.5465688	1.0391254
C	0.4232149	0.7503603	-2.6191902
C	1.4166841	1.5477296	-3.2432736
C	1.1096203	2.3325225	-4.3616439
C	-0.2022105	2.3320446	-4.8574375
C	-1.2107086	1.5617863	-4.2621677
C	-0.8952720	0.7751300	-3.1468047
H	2.4446425	1.5412858	-2.8500957
H	1.8755802	2.9494154	-4.8565640
F	-0.5016656	3.0885787	-5.9302302
H	-2.2287345	1.5845994	-4.6811698
H	-1.6753528	0.1596039	-2.6721317
C	0.7167115	-0.1111110	-1.4981636
C	0.7573191	-1.1846136	-0.8280762
H	0.6802769	-2.2704970	-0.7650598

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.26	0.30305	YES	YES

8	a	22.55	0.21713	YES	YES
9	a	36.75	0.03404	YES	YES
10	a	54.19	0.12635	YES	YES
11	a	68.66	0.12992	YES	YES
12	a	69.04	0.03680	YES	YES
13	a	85.76	1.19921	YES	YES
14	a	89.39	0.32021	YES	YES
15	a	98.28	0.65821	YES	YES
16	a	108.74	0.22748	YES	YES
17	a	111.52	0.15179	YES	YES
18	a	112.93	0.28324	YES	YES
19	a	121.44	0.12117	YES	YES
20	a	139.59	2.64905	YES	YES
21	a	158.76	3.46708	YES	YES
22	a	189.00	1.22604	YES	YES
23	a	214.26	1.85074	YES	YES
24	a	239.50	0.51428	YES	YES
25	a	259.39	6.47716	YES	YES
26	a	264.27	3.68135	YES	YES
27	a	284.68	0.09891	YES	YES
28	a	357.70	3.02508	YES	YES
29	a	378.20	28.05821	YES	YES
30	a	391.70	11.00793	YES	YES
31	a	409.93	0.75986	YES	YES
32	a	415.89	1.48373	YES	YES
33	a	419.65	11.81778	YES	YES
34	a	435.47	6.80079	YES	YES
35	a	451.76	20.06276	YES	YES
36	a	456.40	2.32529	YES	YES
37	a	461.08	1.55757	YES	YES
38	a	477.37	5.21520	YES	YES
39	a	486.93	2.06431	YES	YES
40	a	493.26	5.14778	YES	YES
41	a	502.04	11.11529	YES	YES
42	a	503.59	1.08353	YES	YES
43	a	526.90	38.61188	YES	YES
44	a	538.69	9.57228	YES	YES
45	a	550.87	7.09999	YES	YES
46	a	556.89	1.66527	YES	YES
47	a	609.50	33.01311	YES	YES
48	a	622.64	9.01751	YES	YES
49	a	625.26	5.49474	YES	YES
50	a	630.58	8.65305	YES	YES

2bf'

SCF Energy (au) BP86/SV(P) -2376.684012464
SCF Energy (au) PBE0/def2-TZVPP -2376.261119915
SCF Energy (au) PBE0/def2-TZVPP -2376.2683674155 (Toluene Correction)
Zero Point Energy (au) 0.2819030
Chemical Potential (kJ mol^{-1}) 591.74
Dispersion Correction (au) PBE0/def2-TZVPP -0.06372121

xyz coordinates
41

Mn	1.2369841	1.8112428	0.2458945
C	1.3710057	2.2239260	1.9979497
C	2.9973830	1.4946875	0.1231146
C	1.4070378	3.5547432	-0.2208095
O	1.5385251	4.6804844	-0.5020000
O	4.1374258	1.2590269	0.0458268
O	1.4653967	2.5035421	3.1234923
C	-1.4385143	0.7493141	0.9600496
C	-1.6425046	2.8281922	-0.1147058
C	-3.0389787	2.7999555	-0.0423265
C	-3.6527406	1.6883888	0.5621785
C	-2.8474098	0.6622517	1.0618302
C	-0.4931389	-0.2595865	1.4480186
C	0.8870150	0.0197608	1.2230263
C	1.8292920	-0.9052704	1.7195257
C	1.4267886	-2.0811428	2.3776020
C	0.0601603	-2.3574599	2.5696724
C	-0.8958064	-1.4457124	2.1080509
H	-1.1218721	3.6804176	-0.5784063
H	-3.6263729	3.6366933	-0.4506317
H	-4.7502280	1.6239560	0.6421708
H	-3.3044980	-0.2195121	1.5341995
H	2.9092528	-0.7158254	1.5984144
H	2.1890698	-2.7877433	2.7481177
H	-0.2575013	-3.2783312	3.0851389
H	-1.9647731	-1.6620028	2.2701512
N	-0.8574199	1.8421104	0.3700461
H	1.1178314	2.5991783	-2.6467347
C	1.0251692	1.8237949	-1.8842664
C	0.9074673	0.6019790	-1.5617475
C	0.6359327	-0.7934439	-1.8185723
C	0.0850213	-3.4861763	-2.3995169
C	1.3372732	-3.1407576	-1.8718695
C	1.6054862	-1.7987903	-1.5754792
C	-0.6198875	-1.1771431	-2.3554369
C	-0.8990480	-2.5194103	-2.6455898
F	-0.1785803	-4.7781744	-2.6779051
H	2.0861359	-3.9282089	-1.6949677
H	2.5847550	-1.5154101	-1.1615720
H	-1.3812274	-0.4052900	-2.5485932
H	-1.8699069	-2.8282538	-3.0633400

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.39	0.27467	YES	YES

8	a	21.55	0.51847	YES	YES
9	a	44.50	0.11890	YES	YES
10	a	50.19	0.06929	YES	YES
11	a	63.50	0.12389	YES	YES
12	a	70.81	0.39479	YES	YES
13	a	86.26	0.60158	YES	YES
14	a	93.80	0.51872	YES	YES
15	a	96.25	0.54080	YES	YES
16	a	103.98	0.46765	YES	YES
17	a	111.32	0.04869	YES	YES
18	a	112.85	0.20982	YES	YES
19	a	127.43	0.18839	YES	YES
20	a	148.93	1.14170	YES	YES
21	a	165.79	2.17073	YES	YES
22	a	189.15	0.17288	YES	YES
23	a	218.42	0.44821	YES	YES
24	a	231.41	2.55714	YES	YES
25	a	255.37	1.15210	YES	YES
26	a	271.20	1.74803	YES	YES
27	a	284.92	0.21224	YES	YES
28	a	358.46	2.27539	YES	YES
29	a	382.81	26.61717	YES	YES
30	a	389.11	7.98426	YES	YES
31	a	409.08	0.41539	YES	YES
32	a	411.80	2.83525	YES	YES
33	a	420.64	1.59546	YES	YES
34	a	434.52	4.52181	YES	YES
35	a	448.98	7.51490	YES	YES
36	a	457.87	1.61266	YES	YES
37	a	468.81	5.63922	YES	YES
38	a	476.20	2.44933	YES	YES
39	a	488.08	1.56393	YES	YES
40	a	490.83	1.81398	YES	YES
41	a	499.72	3.43406	YES	YES
42	a	505.68	14.63655	YES	YES
43	a	529.19	23.69735	YES	YES
44	a	535.60	4.82454	YES	YES
45	a	557.17	2.54145	YES	YES
46	a	565.67	3.11213	YES	YES
47	a	613.82	45.67900	YES	YES
48	a	622.84	13.82057	YES	YES
49	a	625.83	15.93175	YES	YES
50	a	629.85	3.56307	YES	YES

2bg

SCF Energy (au) BP86/SV(P) -2614.328819566
SCF Energy (au) PBE0/def2-TZVPP -2613.948640333
SCF Energy (au) PBE0/def2-TZVPP -2613.9559675194 (Toluene Correction)
Zero Point Energy (au) 0.2944290
Chemical Potential (kJ mol^{-1}) 612.46
Dispersion Correction (au) PBE0/def2-TZVPP -0.06476787

xyz coordinates
44

Mn	1.3766062	-0.0299156	1.0645268
C	1.8229581	0.4356415	2.7480525
C	3.0622173	-0.5265104	0.7094753
C	1.6638503	1.6585459	0.4552845
O	1.8874604	2.7516652	0.1141967
O	4.1554677	-0.8631109	0.4807096
O	2.1184501	0.7296068	3.8343661
C	-1.2766004	-0.6795420	2.2218831
C	-1.3620294	1.3794322	1.0940160
C	-2.7193760	1.5530719	1.3844939
C	-3.3748007	0.5573279	2.1295807
C	-2.6482706	-0.5605927	2.5468182
C	-0.4139833	-1.8012923	2.6080498
C	0.9421134	-1.7237824	2.1748488
C	1.8120399	-2.7718873	2.5409442
C	1.3560960	-3.8700920	3.2912667
C	0.0112576	-3.9433639	3.7031411
C	-0.8691605	-2.9102356	3.3632339
H	-0.8122469	2.1383073	0.5159744
H	-3.2432126	2.4549779	1.0324646
H	-4.4429880	0.6539621	2.3839604
H	-3.1391444	-1.3524911	3.1310133
H	2.8717417	-2.7431955	2.2367681
H	2.0593057	-4.6767524	3.5601350
H	-0.3465864	-4.8032959	4.2922161
H	-1.9196367	-2.9708702	3.6924543
N	-0.6527397	0.3016419	1.4946763
C	0.4549691	0.5132800	-2.1782245
C	1.4807382	1.2754454	-2.7931028
C	1.2051413	2.0684467	-3.9116446
C	-0.1007871	2.1280631	-4.4365857
C	-1.1299957	1.3826546	-3.8324164
C	-0.8568091	0.5831906	-2.7158327
H	2.5032306	1.2358872	-2.3878685
H	2.0116705	2.6551033	-4.3782887
C	-0.3766414	2.9532026	-5.6723436
H	-2.1527451	1.4310007	-4.2369787
H	-1.6623480	-0.0018611	-2.2452578
C	0.7144502	-0.3458806	-1.0471444
C	0.7396745	-1.4246914	-0.3831151
H	0.6447374	-2.5096058	-0.3253393
F	0.3742405	4.0809757	-5.7000792
F	-1.6778780	3.3258943	-5.7536733
F	-0.0904370	2.2616444	-6.8066550

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.17	0.41522	YES	YES
8	a	20.39	0.15130	YES	YES
9	a	35.27	0.10531	YES	YES
10	a	37.43	0.03820	YES	YES
11	a	49.21	0.09937	YES	YES
12	a	62.82	0.21459	YES	YES
13	a	69.00	0.07337	YES	YES
14	a	83.96	0.19366	YES	YES
15	a	85.66	1.32995	YES	YES
16	a	92.84	0.36282	YES	YES
17	a	95.29	0.95302	YES	YES
18	a	106.47	0.10456	YES	YES
19	a	109.91	0.10488	YES	YES
20	a	113.97	0.26757	YES	YES
21	a	122.89	0.94308	YES	YES
22	a	152.58	1.00454	YES	YES
23	a	178.29	2.11843	YES	YES
24	a	187.68	2.07863	YES	YES
25	a	204.44	0.65822	YES	YES
26	a	223.75	0.27808	YES	YES
27	a	240.54	0.77371	YES	YES
28	a	260.93	0.55345	YES	YES
29	a	280.59	0.60115	YES	YES
30	a	291.71	0.57093	YES	YES
31	a	320.94	39.44566	YES	YES
32	a	358.15	1.90390	YES	YES
33	a	382.50	3.39938	YES	YES
34	a	397.47	9.23041	YES	YES
35	a	403.54	6.39425	YES	YES
36	a	417.84	10.02122	YES	YES
37	a	429.45	1.95527	YES	YES
38	a	446.92	4.61272	YES	YES
39	a	456.06	1.37970	YES	YES
40	a	456.24	8.85877	YES	YES
41	a	473.87	3.19751	YES	YES
42	a	485.82	2.00936	YES	YES
43	a	491.78	5.65688	YES	YES
44	a	496.06	1.61189	YES	YES
45	a	501.48	5.88190	YES	YES
46	a	515.47	9.01132	YES	YES
47	a	535.60	26.33736	YES	YES
48	a	548.45	5.41518	YES	YES
49	a	556.91	3.03587	YES	YES
50	a	561.76	8.27135	YES	YES

2bg'

SCF Energy (au) BP86/SV(P) -2614.327168892
SCF Energy (au) PBE0/def2-TZVPP -2613.947026262
SCF Energy (au) PBE0/def2-TZVPP -2613.9542738044 (Toluene Correction)
Zero Point Energy (au) 0.2946089
Chemical Potential (kJ mol^{-1}) 615.65
Dispersion Correction (au) PBE0/def2-TZVPP -0.06779443

xyz coordinates
44

Mn	1.2573837	2.1963969	0.4486841
C	1.3531009	2.5665551	2.2135486
C	3.0245241	1.9082488	0.3486739
C	1.4107084	3.9540834	0.0305177
O	1.5310693	5.0887235	-0.2159537
O	4.1686241	1.6910536	0.2840612
O	1.4228473	2.8195984	3.3467836
C	-1.4121583	1.0754608	1.0929445
C	-1.6333439	3.1754795	0.0628049
C	-3.0302405	3.1192127	0.1047146
C	-3.6349183	1.9818055	0.6689859
C	-2.8208450	0.9593536	1.1620807
C	-0.4584825	0.0722705	1.5772752
C	0.9207441	0.3822284	1.3919805
C	1.8703617	-0.5376373	1.8828441
C	1.4759048	-1.7400836	2.4966351
C	0.1110156	-2.0476951	2.6480375
C	-0.8522662	-1.1404826	2.1924812
H	-1.1195922	4.0480721	-0.3696454
H	-3.6251749	3.9540940	-0.2963112
H	-4.7323954	1.8944362	0.7229211
H	-3.2707823	0.0580324	1.6033314
H	2.9487511	-0.3250674	1.7901990
H	2.2430310	-2.4437773	2.8624149
H	-0.2003424	-2.9907485	3.1256045
H	-1.9199092	-1.3831785	2.3217010
N	-0.8401231	2.1925027	0.5405406
H	1.1982519	3.0457681	-2.4312254
C	1.0905043	2.2587945	-1.6825979
C	0.9622207	1.0325429	-1.3807726
C	0.6868258	-0.3602690	-1.6397991
C	0.0939562	-3.0796722	-2.1473174
C	1.3701303	-2.7079213	-1.6823147
C	1.6628496	-1.3646825	-1.4238984
C	-0.5884926	-0.7447573	-2.1270631
C	-0.8805765	-2.0905795	-2.3769088
C	-0.2506350	-4.5380390	-2.3353709
H	2.1393655	-3.4781489	-1.5177800
H	2.6599586	-1.0783748	-1.0571861
H	-1.3505437	0.0288712	-2.3095423
H	-1.8735156	-2.3768497	-2.7570294
F	0.8329323	-5.2770393	-2.6769699
F	-1.1879230	-4.7182721	-3.2986776
F	-0.7528007	-5.0803084	-1.1934013

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.98	0.63488	YES	YES
8	a	24.73	0.22465	YES	YES
9	a	43.41	0.03090	YES	YES
10	a	47.63	0.31629	YES	YES
11	a	49.76	0.06600	YES	YES
12	a	61.87	0.26106	YES	YES
13	a	67.06	0.16659	YES	YES
14	a	82.71	0.48376	YES	YES
15	a	89.55	0.21796	YES	YES
16	a	94.33	0.63058	YES	YES
17	a	98.47	0.91191	YES	YES
18	a	103.09	0.30264	YES	YES
19	a	109.36	0.12101	YES	YES
20	a	118.51	0.23764	YES	YES
21	a	126.63	0.43690	YES	YES
22	a	159.54	0.91062	YES	YES
23	a	184.02	0.14154	YES	YES
24	a	193.52	0.22917	YES	YES
25	a	210.22	0.93389	YES	YES
26	a	217.04	0.33259	YES	YES
27	a	235.08	1.62107	YES	YES
28	a	264.01	0.57022	YES	YES
29	a	282.63	0.22548	YES	YES
30	a	298.91	0.34890	YES	YES
31	a	316.84	22.44646	YES	YES
32	a	358.59	1.90104	YES	YES
33	a	384.74	1.73648	YES	YES
34	a	399.82	0.67506	YES	YES
35	a	402.85	10.35245	YES	YES
36	a	417.48	3.87632	YES	YES
37	a	430.27	2.50205	YES	YES
38	a	438.67	2.11925	YES	YES
39	a	457.39	1.48654	YES	YES
40	a	465.98	1.18742	YES	YES
41	a	470.47	2.76870	YES	YES
42	a	485.67	6.06921	YES	YES
43	a	489.03	1.53234	YES	YES
44	a	497.56	4.15803	YES	YES
45	a	502.00	11.68884	YES	YES
46	a	521.01	4.96104	YES	YES
47	a	528.15	14.73262	YES	YES
48	a	556.28	1.44075	YES	YES
49	a	558.45	2.58503	YES	YES
50	a	566.31	2.08477	YES	YES

2bh

SCF Energy (au) BP86/SV(P) -2505.243220756
SCF Energy (au) PBE0/def2-TZVPP -2504.795978988
SCF Energy (au) PBE0/def2-TZVPP -2504.8052396137 (Toluene Correction)
Zero Point Energy (au) 0.3311844
Chemical Potential (kJ mol^{-1}) 706.41
Dispersion Correction (au) PBE0/def2-TZVPP -0.06732812

xyz coordinates
47

Mn	1.3037687	-0.3393686	1.5642927
C	1.7730387	0.1344454	3.2388633
C	2.9894863	-0.8119268	1.1812376
C	1.5546961	1.3527175	0.9477769
O	1.7573715	2.4484425	0.6023689
O	4.0837222	-1.1330871	0.9345719
O	2.0847189	0.4335773	4.3194731
C	-1.3138688	-1.0269365	2.7797729
C	-1.4579333	1.0217737	1.6394196
C	-2.8103401	1.1770946	1.9618594
C	-3.4317669	0.1781784	2.7313711
C	-2.6784524	-0.9257404	3.1383201
C	-0.4265261	-2.1349737	3.1495659
C	0.9175908	-2.0393267	2.6841830
C	1.8101083	-3.0749629	3.0315404
C	1.3873740	-4.1777526	3.7946080
C	0.0540064	-4.2683357	4.2389227
C	-0.8483498	-3.2481047	3.9178066
H	-0.9341412	1.7839641	1.0418882
H	-3.3566609	2.0677959	1.6155462
H	-4.4945293	0.2610368	3.0119807
H	-3.1425832	-1.7205382	3.7401988
H	2.8618655	-3.0326314	2.7023972
H	2.1077454	-4.9742865	4.0480141
H	-0.2779135	-5.1315735	4.8383119
H	-1.8898483	-3.3223666	4.2718269
N	-0.7224954	-0.0414370	2.0314249
C	0.3817212	0.2025585	-1.6825569
C	1.4305623	0.9225264	-2.3113210
C	1.1772920	1.7120587	-3.4373745
C	-0.1314288	1.8162960	-3.9587425
C	-1.1811545	1.1092983	-3.3339399
C	-0.9323909	0.3121893	-2.2126835
H	2.4533471	0.8470271	-1.9109724
H	1.9984106	2.2594003	-3.9235976
C	-0.4621050	2.6479676	-5.1560877
H	-2.1956412	1.1981318	-3.7536394
H	-1.7525776	-0.2447689	-1.7327883
C	0.6246510	-0.6587717	-0.5500646
C	0.6522165	-1.7324185	0.1221244
H	0.5521967	-2.8167169	0.1840923
O	0.6347577	3.2637250	-5.6739877
O	-1.5811101	2.7704014	-5.6290021
C	0.3952956	4.0772873	-6.8291640
H	1.3816802	4.4905983	-7.1168170
H	-0.3167022	4.8971929	-6.5931624
H	-0.0291043	3.4703400	-7.6578580

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.57	0.40934	YES	YES
8	a	21.74	0.40464	YES	YES
9	a	27.08	1.41359	YES	YES
10	a	46.22	0.15075	YES	YES
11	a	59.22	0.08189	YES	YES
12	a	65.99	0.43548	YES	YES
13	a	72.96	0.34214	YES	YES
14	a	81.48	0.30844	YES	YES
15	a	84.43	1.94921	YES	YES
16	a	90.25	0.19612	YES	YES
17	a	93.42	0.21922	YES	YES
18	a	103.84	0.38580	YES	YES
19	a	109.74	0.07931	YES	YES
20	a	113.53	0.35221	YES	YES
21	a	120.73	0.30032	YES	YES
22	a	125.90	0.91882	YES	YES
23	a	147.48	1.71613	YES	YES
24	a	152.66	4.50491	YES	YES
25	a	177.22	1.29846	YES	YES
26	a	188.89	1.54772	YES	YES
27	a	209.11	1.48568	YES	YES
28	a	234.98	0.55588	YES	YES
29	a	245.53	4.50037	YES	YES
30	a	262.35	0.79599	YES	YES
31	a	283.14	0.95130	YES	YES
32	a	311.13	27.87040	YES	YES
33	a	327.93	11.67023	YES	YES
34	a	350.73	23.39475	YES	YES
35	a	359.49	5.82019	YES	YES
36	a	404.30	0.02491	YES	YES
37	a	416.19	3.06781	YES	YES
38	a	426.53	2.24478	YES	YES
39	a	440.49	1.77115	YES	YES
40	a	449.10	1.71625	YES	YES
41	a	455.95	1.03867	YES	YES
42	a	457.74	24.14923	YES	YES
43	a	473.30	2.85469	YES	YES
44	a	485.96	1.78627	YES	YES
45	a	491.68	6.24711	YES	YES
46	a	501.47	4.97107	YES	YES
47	a	514.16	12.33024	YES	YES
48	a	525.09	28.57055	YES	YES
49	a	538.51	13.49851	YES	YES
50	a	549.73	5.41364	YES	YES

2bh'

SCF Energy (au) BP86/SV(P)	-2505.241127470
SCF Energy (au) PBE0/def2-TZVPP	-2504.793700599
SCF Energy (au) PBE0/def2-TZVPP	-2504.8031262880 (Toluene Correction)
Zero Point Energy (au)	0.3312181
Chemical Potential (kJ mol^{-1})	706.73
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06985329

xyz coordinates

47

Mn	1.3525788	2.6404515	0.6752257
C	1.4623236	3.0505351	2.4306510
C	3.1180559	2.3426824	0.5704972
C	1.5125479	4.3868787	0.2159357
O	1.6366598	5.5146486	-0.0592851
O	4.2612268	2.1210474	0.5048932
O	1.5409259	3.3295203	3.5572676
C	-1.3186215	1.5605827	1.3798475
C	-1.5332292	3.6333060	0.2947321
C	-2.9296576	3.5961481	0.3631720
C	-3.5376511	2.4833359	0.9711769
C	-2.7271811	1.4647459	1.4779097
C	-0.3682498	0.5597142	1.8746643
C	1.0111152	0.8482912	1.6580389
C	1.9583656	-0.0697541	2.1565151
C	1.5609619	-1.2495664	2.8106551
C	0.1954744	-1.5350771	2.9966655
C	-0.7651302	-0.6299190	2.5318795
H	-1.0168526	4.4866881	-0.1716124
H	-3.5214392	4.4269324	-0.0508772
H	-4.6349005	2.4121097	1.0484499
H	-3.1798632	0.5823249	1.9532209
H	3.0373138	0.1269373	2.0393990
H	2.3263312	-1.9524765	3.1813687
H	-0.1177088	-2.4595193	3.5083338
H	-1.8332349	-0.8548593	2.6874203
N	-0.7433560	2.6546985	0.7866600
H	1.2544836	3.4323463	-2.2177885
C	1.1606076	2.6610036	-1.4510573
C	1.0487005	1.4378508	-1.1274324
C	0.8093861	0.0385225	-1.3890164
C	0.3167967	-2.6897427	-1.9836557
C	1.5686989	-2.2825122	-1.4724613
C	1.8129129	-0.9403944	-1.1709397
C	-0.4473827	-0.3759304	-1.9026725
C	-0.6896091	-1.7225133	-2.1952754
C	0.1185604	-4.1403013	-2.2799951
H	2.3449415	-3.0478617	-1.3160285
H	2.7914949	-0.6294426	-0.7751307
H	-1.2314324	0.3781846	-2.0747522
H	-1.6651795	-2.0356814	-2.5961769
O	-1.1267215	-4.4022476	-2.7663730
O	0.9619567	-5.0071900	-2.1138995
C	-1.3865221	-5.7761092	-3.0780381
H	-0.6831782	-6.1448367	-3.8557727
H	-2.4287497	-5.8093542	-3.4516302
H	-1.2765696	-6.4141971	-2.1747089

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.77	0.48046	YES	YES
8	a	16.49	0.07359	YES	YES
9	a	34.31	0.26905	YES	YES
10	a	48.86	0.02328	YES	YES
11	a	55.73	1.09007	YES	YES
12	a	63.10	0.70619	YES	YES
13	a	67.93	0.07690	YES	YES
14	a	82.43	0.35489	YES	YES
15	a	88.48	0.45152	YES	YES
16	a	90.74	0.41964	YES	YES
17	a	96.71	0.40586	YES	YES
18	a	99.94	0.43111	YES	YES
19	a	107.38	0.34149	YES	YES
20	a	114.78	0.64331	YES	YES
21	a	116.87	0.28711	YES	YES
22	a	123.33	0.47748	YES	YES
23	a	151.43	2.54072	YES	YES
24	a	158.10	1.69009	YES	YES
25	a	184.44	0.56521	YES	YES
26	a	191.79	0.56599	YES	YES
27	a	216.79	0.56283	YES	YES
28	a	226.23	2.33570	YES	YES
29	a	241.58	0.48368	YES	YES
30	a	265.96	0.88216	YES	YES
31	a	283.59	0.15454	YES	YES
32	a	310.54	23.14858	YES	YES
33	a	326.65	1.88924	YES	YES
34	a	357.04	8.70207	YES	YES
35	a	361.20	13.57125	YES	YES
36	a	403.29	0.05072	YES	YES
37	a	416.59	9.13494	YES	YES
38	a	422.54	1.21557	YES	YES
39	a	434.43	5.46699	YES	YES
40	a	457.11	2.85989	YES	YES
41	a	458.87	3.97714	YES	YES
42	a	466.11	1.90131	YES	YES
43	a	470.44	2.27312	YES	YES
44	a	486.24	6.29781	YES	YES
45	a	489.75	3.99537	YES	YES
46	a	500.49	2.36214	YES	YES
47	a	508.50	10.92025	YES	YES
48	a	526.16	19.44830	YES	YES
49	a	534.84	2.05306	YES	YES
50	a	556.88	1.91812	YES	YES

2bi

SCF Energy (au) BP86/SV(P)	-2508.412127961
SCF Energy (au) PBE0/def2-TZVPP	-2507.929859714
SCF Energy (au) PBE0/def2-TZVPP	-2507.9381342801 (Toluene Correction)
Zero Point Energy (au)	0.3689319
Chemical Potential (kJ mol^{-1})	802.70
Dispersion Correction (au) PBE0/def2-TZVPP	-0.08008127

xyz coordinates
51

Mn	1.2130299	1.1283460	0.7677901
C	1.7035251	1.6930919	2.4075242
C	2.9060224	0.7196004	0.3489977
C	1.3402844	2.8290054	0.1489828
O	1.4529387	3.9427431	-0.1788935
O	4.0048144	0.4309846	0.0798274
O	2.0398828	2.0723864	3.4558032
C	-1.3170678	0.3238844	2.0891977
C	-1.6520221	2.2439038	0.7770437
C	-3.0119197	2.3031509	1.0993219
C	-3.5366106	1.3238318	1.9611220
C	-2.6842758	0.3326735	2.4536215
C	-0.3319129	-0.6649198	2.5369774
C	0.9908736	-0.4985782	2.0326552
C	1.9782768	-1.4050739	2.4707026
C	1.6657888	-2.4618788	3.3435286
C	0.3502888	-2.6308128	3.8149470
C	-0.6441053	-1.7318737	3.4136953
H	-1.2015770	2.9926609	0.1072473
H	-3.6387367	3.1062909	0.6823404
H	-4.6015919	1.3339608	2.2454455
H	-3.0718391	-0.4473817	3.1247977
H	3.0216985	-1.2941308	2.1310262
H	2.4590368	-3.1596738	3.6619684
H	0.1037007	-3.4586847	4.4994147
H	-1.6710583	-1.8636835	3.7923921
N	-0.8207181	1.2920030	1.2544310
C	0.4207025	1.6500918	-2.5074411
C	1.4867883	2.4143679	-3.0457378
C	1.3169154	3.1360790	-4.2354252
C	0.0808729	3.1232991	-4.9064612
C	-0.9868061	2.3750914	-4.3801494
C	-0.8224232	1.6450879	-3.1936522
H	2.4588884	2.4257396	-2.5283637
H	2.1609446	3.7168114	-4.6429110
H	-0.0496867	3.6969551	-5.8387960
H	-1.9592198	2.3570001	-4.9000822
H	-1.6581221	1.0554551	-2.7841453
C	0.5779432	0.8415585	-1.3142645
C	0.5270337	-0.2875373	-0.7223688
C	0.2609239	-1.7109594	-0.7565203
C	-0.2803551	-4.4856857	-0.9456125
C	1.0329260	-4.0329921	-0.7238185
C	1.3037063	-2.6616307	-0.6212917
C	-1.0599086	-2.1783404	-0.9771882
C	-1.3244028	-3.5529628	-1.0703561
H	-0.4891628	-5.5657011	-1.0214352
H	1.8581302	-4.7581454	-0.6286880
H	2.3329935	-2.3096110	-0.4541603
H	-1.8783950	-1.4475910	-1.0773034
H	-2.3570132	-3.8982063	-1.2457354

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.30	0.22300	YES	YES
8	a	22.06	0.05960	YES	YES
9	a	26.37	0.05122	YES	YES
10	a	29.53	0.26518	YES	YES
11	a	42.86	0.19185	YES	YES
12	a	47.27	0.19769	YES	YES
13	a	58.61	0.22167	YES	YES
14	a	69.78	0.25509	YES	YES
15	a	77.43	0.33119	YES	YES
16	a	86.68	0.52791	YES	YES
17	a	93.21	0.55682	YES	YES
18	a	99.48	0.43536	YES	YES
19	a	110.27	0.03955	YES	YES
20	a	112.40	0.07220	YES	YES
21	a	118.74	0.41670	YES	YES
22	a	128.61	0.09602	YES	YES
23	a	155.09	0.23330	YES	YES
24	a	172.92	0.64525	YES	YES
25	a	184.50	2.96286	YES	YES
26	a	190.36	1.46917	YES	YES
27	a	217.37	2.47697	YES	YES
28	a	227.91	3.62925	YES	YES
29	a	246.59	2.66370	YES	YES
30	a	263.96	0.15492	YES	YES
31	a	285.78	0.04935	YES	YES
32	a	357.97	2.19617	YES	YES
33	a	380.42	15.73501	YES	YES
34	a	396.16	3.45386	YES	YES
35	a	400.56	0.70936	YES	YES
36	a	402.72	0.46689	YES	YES
37	a	419.58	7.53622	YES	YES
38	a	434.67	7.51619	YES	YES
39	a	447.78	18.79443	YES	YES
40	a	455.69	1.81735	YES	YES
41	a	466.54	3.39152	YES	YES
42	a	473.94	4.02064	YES	YES
43	a	487.42	1.59525	YES	YES
44	a	494.62	8.89332	YES	YES
45	a	500.57	40.66585	YES	YES
46	a	510.17	18.38623	YES	YES
47	a	532.27	6.91702	YES	YES
48	a	541.86	10.49425	YES	YES
49	a	546.65	14.41346	YES	YES
50	a	556.32	1.85781	YES	YES

2bj

SCF Energy (au) BP86/SV(P)	-2360.882425609
SCF Energy (au) PBE0/def2-TZVPP	-2360.449384567
SCF Energy (au) PBE0/def2-TZVPP	-2360.4555509522 (Toluene Correction)
Zero Point Energy (au)	0.4312242
Chemical Potential (kJ mol^{-1})	961.18
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07158498

xyz coordinates

55

Mn	0.9063604	1.1654989	1.2513929
C	1.4579883	1.7774516	2.8523784
C	2.5778462	0.7095393	0.8022817
C	1.0471178	2.8159490	0.5310960
O	1.1618663	3.9010142	0.1081574
O	3.6636985	0.3933969	0.5122264
O	1.8356109	2.1749044	3.8800338
C	-1.6068028	0.4517863	2.6622762
C	-1.9209358	2.3794980	1.3603483
C	-3.2626150	2.4940528	1.7393193
C	-3.7889360	1.5380768	2.6254461
C	-2.9554606	0.5154195	3.0851400
C	-0.6429715	-0.5760285	3.0695296
C	0.6614645	-0.4621593	2.5021412
C	1.6210372	-1.4248806	2.8842198
C	1.3013794	-2.4730750	3.7653559
C	0.0050144	-2.5810691	4.3047530
C	-0.9629187	-1.6313920	3.9585385
H	-1.4682090	3.1144091	0.6768561
H	-3.8740846	3.3216238	1.3478960
H	-4.8395069	1.5912199	2.9550566
H	-3.3440641	-0.2459782	3.7769777
H	2.6490455	-1.3666327	2.4885330
H	2.0741428	-3.2123366	4.0379284
H	-0.2459702	-3.3996086	4.9989108
H	-1.9742205	-1.7143196	4.3901050
N	-1.1078899	1.3957218	1.8015117
C	0.1463747	1.6673289	-2.0651955
C	0.2249000	0.8325196	-0.8403622
C	0.1834660	-0.2677396	-0.2129212
C	-0.0838458	-1.7237446	-0.1591217
H	0.8271177	-2.2503474	0.2092813
C	-0.5210201	-2.3071547	-1.5199947
H	-0.8611075	-1.9334766	0.6115687
C	-0.7974492	-3.8183739	-1.4622855
H	0.2702275	-2.0995950	-2.2773694
H	-1.4349885	-1.7730181	-1.8707999
C	-1.2269150	-4.4107003	-2.8113143
H	-1.5858337	-4.0181631	-0.6987829
H	0.1167171	-4.3439965	-1.0984921
H	-1.4183266	-5.5036238	-2.7325177
H	-0.4421516	-4.2618467	-3.5870862
H	-2.1600508	-3.9322296	-3.1856164
C	1.5045309	1.8713812	-2.7748815
H	-0.5587833	1.1609294	-2.7667554
H	-0.2988621	2.6637806	-1.8441008
H	2.2194946	2.3506684	-2.0687930
C	1.3891197	2.7256069	-4.0470473
H	1.9342444	0.8736357	-3.0233639
C	2.7307898	2.9294680	-4.7625803
H	0.9547438	3.7182795	-3.7817327
H	0.6615254	2.2502414	-4.7469750

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H     3.4687910    3.4359572   -4.1005359
H     2.6138692    3.5544444   -5.6753434
H     3.1754356    1.9576868   -5.0752911

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             11.02         0.17245       YES     YES
     8        a             25.23         0.14043       YES     YES
     9        a             27.66         0.17493       YES     YES
    10        a             40.79         0.02801       YES     YES
    11        a             48.69         0.22577       YES     YES
    12        a             55.13         0.08372       YES     YES
    13        a             61.84         0.07792       YES     YES
    14        a             63.89         0.05944       YES     YES
    15        a             73.91         0.05961       YES     YES
    16        a             84.70         0.87413       YES     YES
    17        a             86.28         0.56138       YES     YES
    18        a             91.79         0.23567       YES     YES
    19        a            101.15         0.08415       YES     YES
    20        a            105.03         0.28350       YES     YES
    21        a            105.92         0.16061       YES     YES
    22        a            115.10         0.13407       YES     YES
    23        a            123.42         0.37657       YES     YES
    24        a            127.51         0.13969       YES     YES
    25        a            134.65         0.14269       YES     YES
    26        a            167.09         1.19662       YES     YES
    27        a            185.09         1.62408       YES     YES
    28        a            192.02         1.72794       YES     YES
    29        a            207.29         0.25131       YES     YES
    30        a            212.04         0.94338       YES     YES
    31        a            230.67         0.44577       YES     YES
    32        a            245.13         0.09361       YES     YES
    33        a            251.99         0.09030       YES     YES
    34        a            257.44         0.71190       YES     YES
    35        a            284.92         0.04044       YES     YES
    36        a            287.84         1.99290       YES     YES
    37        a            342.65         1.35575       YES     YES
    38        a            351.28        10.47142       YES     YES
    39        a            358.57         2.50273       YES     YES
    40        a            377.52         7.71193       YES     YES
    41        a            413.42         0.40739       YES     YES
    42        a            417.98         3.93799       YES     YES
    43        a            436.39         0.17315       YES     YES
    44        a            456.70         1.43676       YES     YES
    45        a            459.24         3.11548       YES     YES
    46        a            472.34         2.92312       YES     YES
    47        a            487.20         4.26455       YES     YES
    48        a            493.34         0.83376       YES     YES
    49        a            504.92         1.30037       YES     YES
    50        a            511.34         0.08654       YES     YES
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SCF Energy (au) BP86/SV(P) -2678.190493143
SCF Energy (au) PBE0/def2-TZVPP -2677.706850638
SCF Energy (au) PBE0/def2-TZVPP -2677.7183769724 (Toluene Correction)
Zero Point Energy (au) 0.4157036
Chemical Potential (kJ mol^{-1}) 911.24
Dispersion Correction (au) PBE0/def2-TZVPP -0.08425883

xyz coordinates
57

Mn	0.7905336	1.5285988	-0.7423591
C	1.3273161	1.7047316	0.9650669
C	2.4456986	0.9692036	-1.2253026
C	1.2218679	3.2420649	-1.1491495
O	1.5213430	4.3518560	-1.3572636
O	3.5159990	0.7182341	-1.6022172
O	1.6847253	1.7901848	2.0709940
C	-1.9172557	1.0193716	0.3528721
C	-1.7957953	3.1873913	-0.5318246
C	-3.1303060	3.4572047	-0.2048991
C	-3.8817482	2.4552653	0.4318321
C	-3.2678746	1.2300441	0.7097169
C	-1.1664315	-0.2164499	0.5949210
C	0.1556683	-0.2054871	0.1489748
C	0.9967886	-1.3733598	0.3826172
N	0.3757456	-2.4857002	1.0476719
C	-0.9469338	-2.4827290	1.4670707
C	-1.7248080	-1.3636875	1.2467454
H	-1.1767336	3.9503746	-1.0275713
H	-3.5624970	4.4401795	-0.4476092
H	-4.9345600	2.6283193	0.7088086
H	-3.8313851	0.4263969	1.2057034
O	2.1917129	-1.4589280	0.0571630
C	-1.4998894	-3.7096034	2.1450369
H	-2.7692106	-1.3801603	1.5893197
N	-1.1933158	2.0084472	-0.2649113
C	-0.2026858	2.5515868	-3.8505661
C	0.8330593	3.3355169	-4.4204606
C	0.5392223	4.3032118	-5.3907774
C	-0.7879149	4.5174378	-5.8053061
C	-1.8237181	3.7496072	-5.2446583
C	-1.5387683	2.7755920	-4.2763370
H	1.8734261	3.1710737	-4.0999638
H	1.3574875	4.8993708	-5.8272260
H	-1.0141382	5.2828874	-6.5658297
H	-2.8665484	3.9080653	-5.5667153
H	-2.3482659	2.1684774	-3.8410303
C	0.0717449	1.5172662	-2.8807799
C	0.0979632	0.3619270	-2.3637414
H	-0.0035840	-0.7198586	-2.4531376
H	-1.5173194	-4.5908682	1.4635559
H	-2.5420262	-3.5195711	2.4730421
H	-0.9011095	-3.9959174	3.0374664
C	1.2519414	-3.6507605	1.2827453
C	1.8231970	-3.7377665	2.6904001
H	2.0819419	-3.5235044	0.5560890
H	0.7002069	-4.5790914	1.0321895
C	2.9472178	-3.9354974	5.2820534
C	2.3163704	-5.0476178	4.7009390
C	1.7566335	-4.9455809	3.4153647
C	2.4693801	-2.6285701	3.2789892
C	3.0218256	-2.7272481	4.5658847

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H     3.3831164   -4.0094872    6.2921715
H     2.2541763   -6.0011177    5.2516107
H     1.2615839   -5.8247528    2.9659924
H     2.5537513   -1.6850764    2.7160355
H     3.5231786   -1.8514973    5.0105932

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             11.75         0.05816       YES     YES
     8        a             14.17         0.44665       YES     YES
     9        a             18.27         0.27503       YES     YES
    10        a             25.24         0.43345       YES     YES
    11        a             28.41         0.17720       YES     YES
    12        a             33.39         0.16288       YES     YES
    13        a             52.56         2.02624       YES     YES
    14        a             61.46         0.06639       YES     YES
    15        a             70.66         0.31006       YES     YES
    16        a             77.87         0.45878       YES     YES
    17        a             82.82         0.65931       YES     YES
    18        a             91.77         2.72653       YES     YES
    19        a             98.13         0.53621       YES     YES
    20        a            101.45         0.06260       YES     YES
    21        a            111.21         0.12231       YES     YES
    22        a            118.61         0.89381       YES     YES
    23        a            121.91         1.04289       YES     YES
    24        a            152.08         0.91687       YES     YES
    25        a            152.54         0.72509       YES     YES
    26        a            160.88         4.90822       YES     YES
    27        a            183.22         0.71152       YES     YES
    28        a            194.04         1.37194       YES     YES
    29        a            208.22         1.82511       YES     YES
    30        a            222.93         0.28827       YES     YES
    31        a            244.70         1.18420       YES     YES
    32        a            247.38         0.73847       YES     YES
    33        a            261.67         1.67246       YES     YES
    34        a            279.46         0.50349       YES     YES
    35        a            311.39         3.41575       YES     YES
    36        a            323.37        15.15492       YES     YES
    37        a            333.50        13.91151       YES     YES
    38        a            369.01         6.10197       YES     YES
    39        a            388.19         1.01913       YES     YES
    40        a            401.34         0.06661       YES     YES
    41        a            402.35         0.33753       YES     YES
    42        a            416.94        18.50278       YES     YES
    43        a            429.83         3.80817       YES     YES
    44        a            439.12        14.05357       YES     YES
    45        a            455.41         8.65813       YES     YES
    46        a            462.46        13.72343       YES     YES
    47        a            465.15         2.29291       YES     YES
    48        a            470.80         0.71839       YES     YES
    49        a            479.01         8.66726       YES     YES
    50        a            486.70         6.50033       YES     YES
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SCF Energy (au) BP86/SV(P)	-2678.190378706	
SCF Energy (au) PBE0/def2-TZVPP	-2677.706376595	
SCF Energy (au) PBE0/def2-TZVPP	-2677.7174819824	(Toluene Correction)
Zero Point Energy (au)	0.4159746	
Chemical Potential (kJ mol^{-1})	916.06	
Dispersion Correction (au) PBE0/def2-TZVPP	-0.08639897	

xyz coordinates
57

Mn	0.7961401	2.5847105	-1.0851902
C	1.2500491	2.7717503	0.6500830
C	2.4813310	2.0544182	-1.5070732
C	1.1939145	4.3117903	-1.4411958
O	1.4534377	5.4315807	-1.6517531
O	3.5663854	1.8259195	-1.8522930
O	1.5603437	2.8875984	1.7671783
C	-1.9187337	1.9701171	-0.0555799
C	-1.8776272	4.1124029	-1.0050859
C	-3.2343521	4.3236173	-0.7320304
C	-3.9555682	3.3032904	-0.0892464
C	-3.2903241	2.1206326	0.2481533
C	-1.1141102	0.7822773	0.2480661
C	0.2167596	0.8397673	-0.1695494
C	1.1073012	-0.2669546	0.1537331
N	0.5226619	-1.3819293	0.8429219
C	-0.8113962	-1.4330731	1.2170725
C	-1.6355385	-0.3635921	0.9287325
H	-1.2791530	4.8905777	-1.5034612
H	-3.7078776	5.2752248	-1.0190629
H	-5.0252499	3.4288905	0.1451857
H	-3.8303504	1.3024026	0.7462112
O	2.3204438	-0.3020275	-0.1188913
C	-1.3260705	-2.6620627	1.9203533
H	-2.6889701	-0.4207582	1.2375034
N	-1.2260492	2.9768015	-0.6777181
H	0.4305322	3.6470920	-3.8642917
C	0.3284714	2.8248482	-3.1539352
C	0.1072887	1.5993603	-2.8967459
C	-0.3320158	0.2701243	-3.2666099
H	-1.2831841	-3.5629399	1.2663069
H	-2.3851514	-2.5114458	2.2126235
H	-0.7412688	-2.8920748	2.8379881
C	1.4470592	-2.4902952	1.1537664
C	1.9717429	-2.4950662	2.5821842
H	2.2958274	-2.3481379	0.4523575
H	0.9511891	-3.4540546	0.9211390
C	3.0186002	-2.5396166	5.2130484
C	2.4738845	-3.7060846	4.6516553
C	1.9522292	-3.6802039	3.3463164
C	2.5307111	-1.3301185	3.1518695
C	3.0448033	-1.3531060	4.4581470
H	3.4249358	-2.5541871	6.2379724
H	2.4496076	-4.6430481	5.2327775
H	1.5253732	-4.6016461	2.9121475
H	2.5769806	-0.4018958	2.5601036
H	3.4779642	-0.4344876	4.8877950
C	-1.1888456	-2.2916190	-4.1159708
C	-2.0009716	-1.1662434	-4.3406083
C	-1.5782448	0.1047369	-3.9237175
C	0.4736494	-0.8723298	-3.0325241
C	0.0486945	-2.1367172	-3.4651808

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H    -1.5195209   -3.2892602   -4.4495344
H    -2.9725869   -1.2768177   -4.8508210
H    -2.2099208    0.9891133   -4.1055410
H     1.4407025   -0.7534001   -2.5191253
H     0.6940667   -3.0138514   -3.2906557

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             13.98         0.16013       YES     YES
     8        a             18.45         0.16169       YES     YES
     9        a             23.39         0.91198       YES     YES
    10        a             26.84         0.00583       YES     YES
    11        a             34.42         0.15750       YES     YES
    12        a             49.10         0.02982       YES     YES
    13        a             52.96         1.01254       YES     YES
    14        a             63.51         0.73153       YES     YES
    15        a             73.89         0.63088       YES     YES
    16        a             79.38         0.96375       YES     YES
    17        a             82.15         1.07061       YES     YES
    18        a             95.65         0.70579       YES     YES
    19        a            100.84         0.36578       YES     YES
    20        a            104.48         0.08703       YES     YES
    21        a            109.67         0.84019       YES     YES
    22        a            122.89         1.57095       YES     YES
    23        a            128.37         0.61223       YES     YES
    24        a            153.86         0.54673       YES     YES
    25        a            158.56         0.16737       YES     YES
    26        a            178.88         0.53684       YES     YES
    27        a            185.41         2.14388       YES     YES
    28        a            192.23         1.63138       YES     YES
    29        a            206.72         1.76481       YES     YES
    30        a            213.42         0.34350       YES     YES
    31        a            243.95         1.05407       YES     YES
    32        a            247.83         1.08144       YES     YES
    33        a            262.98         0.36073       YES     YES
    34        a            281.31         1.23538       YES     YES
    35        a            310.09         5.88444       YES     YES
    36        a            330.66         9.26868       YES     YES
    37        a            342.45         5.75582       YES     YES
    38        a            367.77         4.50765       YES     YES
    39        a            391.01         1.25030       YES     YES
    40        a            402.56         0.10780       YES     YES
    41        a            403.68         2.37536       YES     YES
    42        a            409.01        13.17384       YES     YES
    43        a            431.49        11.95146       YES     YES
    44        a            442.41        14.97434       YES     YES
    45        a            457.92         0.40690       YES     YES
    46        a            464.95         1.20181       YES     YES
    47        a            468.56         6.69897       YES     YES
    48        a            471.25         3.35441       YES     YES
    49        a            478.00         3.89641       YES     YES
    50        a            485.52         6.40456       YES     YES
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2da

SCF Energy (au) BP86/SV(P) -2409.004534403
SCF Energy (au) PBE0/def2-TZVPP -2408.542817634
SCF Energy (au) PBE0/def2-TZVPP -2408.5510777761 (Toluene Correction)
Zero Point Energy (au) 0.3178444
Chemical Potential (kJ mol^{-1}) 679.64
Dispersion Correction (au) PBE0/def2-TZVPP -0.06709809

xyz coordinates
45

Mn	1.5197310	0.5470025	0.3436074
C	1.9098030	0.8269867	2.0810763
C	3.1834914	-0.0444268	0.0203656
C	1.9301135	2.2698775	-0.0671300
O	2.2237609	3.3814057	-0.2662464
O	4.2544275	-0.4565929	-0.1836553
O	2.1616682	1.0008020	3.2032102
C	-1.2049045	-0.1258313	1.2768286
C	-1.1589754	2.0562942	0.4177521
C	-2.5219656	2.2484819	0.6575306
C	-3.2447226	1.1885736	1.2332793
C	-2.5904925	-0.0046829	1.5445731
N	-0.4345005	-1.2439296	1.5412602
C	0.9499691	-1.2028048	1.1921142
C	1.5082306	-2.4082537	1.5598700
C	0.4804587	-3.2427178	2.1402405
C	-0.7448065	-2.4960049	2.1266952
H	-0.5477021	2.8540095	-0.0310344
H	-2.9972974	3.2064907	0.3991233
H	-4.3222679	1.2891001	1.4423592
H	-3.1456491	-0.8365420	1.9889839
H	2.5624864	-2.6854686	1.4310032
C	0.4951000	-4.5502559	2.6685547
N	-0.5072941	0.9101560	0.7131965
C	0.8271748	1.5978722	-2.8620085
C	1.9509091	2.3147130	-3.3463859
C	1.7939842	3.2932883	-4.3372283
C	0.5191695	3.5832855	-4.8561966
C	-0.6026395	2.8814165	-4.3811110
C	-0.4550859	1.8969480	-3.3931721
H	2.9505721	2.0905373	-2.9429216
H	2.6781598	3.8380295	-4.7070955
H	0.4001929	4.3572543	-5.6321738
H	-1.6046992	3.1003949	-4.7859256
H	-1.3312893	1.3404153	-3.0245511
C	0.9579810	0.5504308	-1.8770337
C	0.8890639	-0.5923575	-1.3453656
H	0.7411585	-1.6707348	-1.3980957
H	1.4336625	-5.1283198	2.6819725
C	-0.6914407	-5.1000768	3.1740729
H	-0.6902216	-6.1214082	3.5892289
C	-1.8900312	-4.3559507	3.1584690
H	-2.8156297	-4.7983334	3.5616334
C	-1.9319458	-3.0495780	2.6376779
H	-2.8877072	-2.5094957	2.6526528

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.31	0.07965	YES	YES
8	a	17.65	0.09997	YES	YES
9	a	25.65	0.26847	YES	YES
10	a	47.19	0.24354	YES	YES
11	a	56.47	0.07018	YES	YES
12	a	64.10	0.09528	YES	YES
13	a	67.11	0.32495	YES	YES
14	a	79.62	0.42679	YES	YES
15	a	87.94	0.74734	YES	YES
16	a	99.82	0.51131	YES	YES
17	a	104.85	1.07356	YES	YES
18	a	111.88	0.11920	YES	YES
19	a	122.33	0.21282	YES	YES
20	a	143.47	1.40069	YES	YES
21	a	157.32	5.11267	YES	YES
22	a	168.97	2.48278	YES	YES
23	a	178.12	0.99525	YES	YES
24	a	215.31	0.22371	YES	YES
25	a	238.99	0.23718	YES	YES
26	a	256.73	6.23442	YES	YES
27	a	280.88	0.52625	YES	YES
28	a	306.39	21.32459	YES	YES
29	a	315.88	1.87150	YES	YES
30	a	352.24	1.47949	YES	YES
31	a	366.05	5.07142	YES	YES
32	a	400.09	0.38943	YES	YES
33	a	407.71	7.20090	YES	YES
34	a	422.47	1.06470	YES	YES
35	a	431.12	1.93796	YES	YES
36	a	456.79	15.18417	YES	YES
37	a	473.69	2.51350	YES	YES
38	a	478.93	13.77269	YES	YES
39	a	486.33	3.55622	YES	YES
40	a	493.78	13.48945	YES	YES
41	a	501.81	16.05292	YES	YES
42	a	513.21	1.64317	YES	YES
43	a	516.95	0.49905	YES	YES
44	a	523.19	37.80879	YES	YES
45	a	537.83	7.06320	YES	YES
46	a	554.10	7.08855	YES	YES
47	a	571.12	0.17654	YES	YES
48	a	589.91	8.62866	YES	YES
49	a	611.07	12.74284	YES	YES
50	a	613.67	2.03699	YES	YES

2da'

SCF Energy (au) BP86/SV(P) -2409.003236277
SCF Energy (au) PBE0/def2-TZVPP -2408.541068212
SCF Energy (au) PBE0/def2-TZVPP -2408.5491894788 (Toluene Correction)
Zero Point Energy (au) 0.3178436
Chemical Potential (kJ mol^{-1}) 680.78
Dispersion Correction (au) PBE0/def2-TZVPP -0.06958346

xyz coordinates
45

Mn	1.6114787	2.0224123	-0.1294482
C	1.9124242	2.3882443	1.6130026
C	3.3069043	1.4797935	-0.3640030
C	1.9537395	3.7493582	-0.5687954
O	2.1911893	4.8621185	-0.8290349
O	4.3945181	1.0868426	-0.5076838
O	2.1133826	2.6348062	2.7313371
C	-1.0999543	1.1950939	0.7151392
C	-1.1734098	3.3233061	-0.2672068
C	-2.5598082	3.4139375	-0.1227346
C	-3.2331398	2.3243121	0.4589504
C	-2.5076960	1.2075558	0.8767864
N	-0.2598291	0.1667125	1.0975266
C	1.1285164	0.2877215	0.7892940
C	1.7639615	-0.8264179	1.2966744
C	0.7824824	-1.6835292	1.9209497
C	-0.4947175	-1.0432808	1.7940818
H	-0.5986462	4.1430608	-0.7250315
H	-3.0927997	4.3144785	-0.4625970
H	-4.3280388	2.3403880	0.5843860
H	-3.0244406	0.3456729	1.3111972
H	2.8428089	-1.0225844	1.2437251
C	0.8787449	-2.9251389	2.5820625
N	-0.4526673	2.2542483	0.1355482
H	1.4252327	2.9305479	-2.9825719
C	1.2749429	2.1317796	-2.2549764
C	1.0302276	0.9214792	-1.9744502
C	0.6010528	-0.4326949	-2.2310418
H	1.8581874	-3.4207374	2.6835846
C	-0.2794590	-3.5132887	3.1097021
H	-0.2150666	-4.4835600	3.6292674
C	-1.5294780	-2.8709534	2.9860483
H	-2.4316533	-3.3406685	3.4109535
C	-1.6528098	-1.6320255	2.3307129
H	-2.6452131	-1.1660218	2.2707994
C	-0.2569970	-3.0608890	-2.8308959
C	-1.1188276	-1.9713558	-3.0487209
C	-0.6974520	-0.6670022	-2.7534160
C	1.4590036	-1.5386594	-2.0074787
C	1.0315616	-2.8379490	-2.3143524
H	-0.5904122	-4.0856771	-3.0632895
H	-2.1299911	-2.1378258	-3.4561038
H	-1.3683259	0.1890256	-2.9296280
H	2.4680464	-1.3648277	-1.6056212
H	1.7124272	-3.6878085	-2.1426469

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.45	0.16430	YES	YES
8	a	20.66	0.16312	YES	YES
9	a	27.61	0.30383	YES	YES
10	a	49.13	0.08630	YES	YES
11	a	59.94	0.16090	YES	YES
12	a	65.57	0.28800	YES	YES
13	a	68.58	0.53915	YES	YES
14	a	75.86	0.08201	YES	YES
15	a	88.40	0.25179	YES	YES
16	a	98.66	0.56138	YES	YES
17	a	103.05	0.65599	YES	YES
18	a	106.88	0.54148	YES	YES
19	a	126.59	0.02338	YES	YES
20	a	150.94	0.53832	YES	YES
21	a	162.96	2.42157	YES	YES
22	a	168.46	1.32486	YES	YES
23	a	178.57	1.51189	YES	YES
24	a	212.26	0.21873	YES	YES
25	a	238.54	0.76712	YES	YES
26	a	257.32	1.47958	YES	YES
27	a	283.38	3.04667	YES	YES
28	a	310.87	5.24429	YES	YES
29	a	327.36	9.96005	YES	YES
30	a	352.85	0.86261	YES	YES
31	a	366.38	4.12868	YES	YES
32	a	398.02	4.32884	YES	YES
33	a	402.62	7.57207	YES	YES
34	a	421.35	4.23673	YES	YES
35	a	430.23	9.78177	YES	YES
36	a	461.07	5.52510	YES	YES
37	a	475.56	2.62213	YES	YES
38	a	479.33	5.02750	YES	YES
39	a	488.60	0.62185	YES	YES
40	a	494.56	6.21874	YES	YES
41	a	497.45	14.72589	YES	YES
42	a	511.89	1.50073	YES	YES
43	a	519.62	1.34959	YES	YES
44	a	529.49	16.84794	YES	YES
45	a	534.71	3.87538	YES	YES
46	a	567.27	4.37452	YES	YES
47	a	571.42	0.03474	YES	YES
48	a	592.92	6.68595	YES	YES
49	a	611.93	9.00493	YES	YES
50	a	613.42	6.37682	YES	YES

2ea

SCF Energy (au) BP86/SV(P)	-2583.758694363
SCF Energy (au) PBE0/def2-TZVPP	-2583.308834131
SCF Energy (au) PBE0/def2-TZVPP	-2583.3186219410 (Toluene Correction)
Zero Point Energy (au)	0.3858375
Chemical Potential (kJ mol^{-1})	840.51
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07229098

xyz coordinates

53

Mn	2.2230988	0.6317792	-0.0380673
C	2.6156062	1.1476731	1.6392340
C	3.9387085	0.1811112	-0.3247176
C	2.4125292	2.3193182	-0.6911169
O	2.5413774	3.4196005	-1.0551924
O	5.0506470	-0.1331539	-0.4981009
O	2.8767051	1.4700797	2.7277647
C	-0.4539945	-0.0297274	0.9096872
C	-1.9246317	0.0913870	1.0871830
C	0.3558878	-1.1297064	1.4172808
C	1.7432603	-1.0509487	1.0754004
C	2.6077351	-2.0542027	1.5517480
C	2.1177715	-3.1166002	2.3474416
C	0.7427944	-3.1752783	2.6929163
C	-0.1235398	-2.1864952	2.2356941
H	3.6801806	-2.0058785	1.3091043
O	2.8869000	-4.1224309	2.8426613
H	0.3950079	-4.0008383	3.3326722
H	-1.1848113	-2.2197783	2.5316610
N	0.2295362	0.8918881	0.2643551
C	1.2662731	1.0751896	-3.2954025
C	2.2345091	1.8668127	-3.9638754
C	1.8687155	2.6586890	-5.0606656
C	0.5347223	2.6874656	-5.5058725
C	-0.4352712	1.9114622	-4.8473054
C	-0.0776139	1.1120552	-3.7519775
H	3.2792071	1.8489973	-3.6164200
H	2.6348500	3.2643171	-5.5724379
H	0.2515102	3.3164568	-6.3659739
H	-1.4830307	1.9265356	-5.1911149
H	-0.8346306	0.4992213	-3.2369763
C	1.6163849	0.2176182	-2.1884952
C	1.7524455	-0.8361841	-1.5029239
H	1.7703661	-1.9228945	-1.4187534
C	-4.7416295	0.3982927	1.3390996
C	-4.1874919	-0.8306805	0.9085777
C	-2.8044347	-0.9812409	0.7916161
C	-2.4915732	1.3143236	1.5082184
C	-3.8796569	1.4757364	1.6412510
O	-6.0976318	0.4422766	1.4283706
H	-4.8744120	-1.6562320	0.6648427
H	-2.3950795	-1.9390571	0.4327292
H	-1.8296331	2.1579555	1.7662896
H	-4.2759343	2.4409076	1.9886844
H	-0.3377541	1.6556536	-0.1300338
C	-6.7187729	1.6476577	1.8463775
H	-6.4076413	1.9356514	2.8783423
H	-7.8093098	1.4493254	1.8391284
H	-6.4964900	2.4895023	1.1487841
C	4.2807820	-4.1239894	2.5719257
H	4.7805171	-3.2159617	2.9829648
H	4.4885289	-4.1896897	1.4784253

H 4.6884108 -5.0239717 3.0749915

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.66	0.11198	YES	YES
8	a	23.85	0.14135	YES	YES
9	a	28.24	0.19019	YES	YES
10	a	35.42	0.79697	YES	YES
11	a	38.32	0.42459	YES	YES
12	a	47.51	0.69116	YES	YES
13	a	61.68	0.10633	YES	YES
14	a	65.84	0.17130	YES	YES
15	a	75.47	0.44825	YES	YES
16	a	85.53	1.07252	YES	YES
17	a	87.59	0.33363	YES	YES
18	a	94.62	0.20706	YES	YES
19	a	101.89	0.26170	YES	YES
20	a	103.56	2.42543	YES	YES
21	a	114.60	0.52142	YES	YES
22	a	121.22	1.35366	YES	YES
23	a	146.22	0.28143	YES	YES
24	a	154.04	1.68102	YES	YES
25	a	160.20	0.18190	YES	YES
26	a	168.67	8.51326	YES	YES
27	a	180.21	2.01157	YES	YES
28	a	190.96	1.43101	YES	YES
29	a	204.10	0.46082	YES	YES
30	a	236.74	0.90063	YES	YES
31	a	246.28	0.61014	YES	YES
32	a	256.47	2.28427	YES	YES
33	a	266.71	1.10966	YES	YES
34	a	300.24	1.39938	YES	YES
35	a	316.99	24.15601	YES	YES
36	a	319.55	2.82845	YES	YES
37	a	342.78	0.96020	YES	YES
38	a	361.53	5.33052	YES	YES
39	a	400.11	0.10893	YES	YES
40	a	409.14	5.85992	YES	YES
41	a	415.96	2.75722	YES	YES
42	a	422.26	1.54838	YES	YES
43	a	444.19	13.52271	YES	YES
44	a	454.37	1.42207	YES	YES
45	a	458.56	2.83272	YES	YES
46	a	475.83	3.34516	YES	YES
47	a	478.06	8.31028	YES	YES
48	a	488.23	4.80640	YES	YES
49	a	495.22	10.53210	YES	YES
50	a	502.27	14.32391	YES	YES

2ea'

SCF Energy (au) BP86/SV(P) -2583.755936542
SCF Energy (au) PBE0/def2-TZVPP -2583.306604497
SCF Energy (au) PBE0/def2-TZVPP -2583.3161494270 (Toluene Correction)
Zero Point Energy (au) 0.3858163
Chemical Potential (kJ mol^{-1}) 841.85
Dispersion Correction (au) PBE0/def2-TZVPP -0.07594655

xyz coordinates
53

Mn	1.9919400	1.9445815	-0.2125446
C	2.1534808	2.3744254	1.5290994
C	3.7492214	1.5853193	-0.3113953
C	2.1488295	3.6785107	-0.7263564
O	2.2404524	4.7993586	-1.0377011
O	4.8853661	1.3177075	-0.3697285
O	2.2698990	2.6577750	2.6525923
C	-0.7159006	1.1112818	0.4928948
C	0.1043036	0.0054276	0.9687169
C	1.5091645	0.1721588	0.7533872
C	2.3773587	-0.8410027	1.1958039
C	1.8728113	-2.0152812	1.8030053
C	0.4752568	-2.1871422	1.9748359
C	-0.3961908	-1.1855143	1.5574072
H	3.4624674	-0.7284284	1.0533317
O	2.6454017	-3.0414031	2.2472929
H	0.1110908	-3.1192603	2.4333817
H	-1.4825776	-1.3313196	1.6747097
N	-0.0377682	2.0698256	-0.1025837
H	1.6963008	2.6226932	-3.1216314
C	1.7555164	1.8524320	-2.3511876
C	1.7682332	0.6340095	-2.0105774
C	1.8077286	-0.8002035	-2.1790042
C	1.9200425	-3.6011320	-2.5779877
C	3.0989686	-2.8350822	-2.6115416
C	3.0485007	-1.4479013	-2.4103047
C	0.6263831	-1.5815302	-2.1436240
C	0.6864749	-2.9683920	-2.3432424
H	1.9626934	-4.6916637	-2.7344687
H	4.0704284	-3.3222218	-2.7994052
H	3.9712861	-0.8468055	-2.4342545
H	-0.3402928	-1.0879230	-1.9607610
H	-0.2421060	-3.5621325	-2.3141260
C	-2.1920915	1.1993839	0.6436670
C	-5.0083214	1.4914085	0.9169598
C	-4.2119099	1.1238512	2.0274378
C	-2.8306057	0.9750933	1.8900714
C	-2.9975772	1.5734107	-0.4539791
C	-4.3889449	1.7150685	-0.3325568
O	-6.3429842	1.6032685	1.1508950
H	-4.7089911	0.9678227	2.9977093
H	-2.2261438	0.7135808	2.7732747
H	-2.5283966	1.7355727	-1.4391278
H	-4.9787167	1.9923799	-1.2184360
H	-0.6034216	2.8775078	-0.3994740
C	-7.1972825	1.9790936	0.0823794
H	-7.1680455	1.2368679	-0.7501530
H	-6.9375345	2.9876305	-0.3178743
H	-8.2215719	2.0095391	0.5047845
C	4.0556463	-2.9552201	2.1058369
H	4.4730160	-2.0857501	2.6654880
H	4.3560879	-2.8782928	1.0352177

H 4.4630239 -3.8933836 2.5338468

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.75	0.06828	YES	YES
8	a	28.47	0.19583	YES	YES
9	a	33.94	0.28112	YES	YES
10	a	36.54	0.25294	YES	YES
11	a	38.48	0.16597	YES	YES
12	a	49.80	1.04111	YES	YES
13	a	54.04	0.26221	YES	YES
14	a	64.84	0.11492	YES	YES
15	a	76.74	0.35850	YES	YES
16	a	84.30	1.11652	YES	YES
17	a	89.15	0.20915	YES	YES
18	a	93.26	0.14079	YES	YES
19	a	96.89	1.50910	YES	YES
20	a	107.51	0.21592	YES	YES
21	a	113.30	0.33480	YES	YES
22	a	120.74	2.23271	YES	YES
23	a	149.98	1.82201	YES	YES
24	a	158.02	1.52750	YES	YES
25	a	163.84	1.18213	YES	YES
26	a	175.37	3.19118	YES	YES
27	a	176.20	2.30265	YES	YES
28	a	183.71	0.31709	YES	YES
29	a	192.21	0.53953	YES	YES
30	a	242.22	0.72845	YES	YES
31	a	249.25	0.73961	YES	YES
32	a	255.05	0.48763	YES	YES
33	a	268.62	1.23736	YES	YES
34	a	296.84	2.72505	YES	YES
35	a	305.94	17.11122	YES	YES
36	a	317.81	1.02634	YES	YES
37	a	340.78	0.34148	YES	YES
38	a	362.30	4.98498	YES	YES
39	a	398.05	10.51671	YES	YES
40	a	399.04	1.53104	YES	YES
41	a	415.91	3.33119	YES	YES
42	a	420.81	0.98381	YES	YES
43	a	444.89	0.66886	YES	YES
44	a	454.90	1.69616	YES	YES
45	a	461.02	2.68253	YES	YES
46	a	479.34	5.64347	YES	YES
47	a	484.40	10.14586	YES	YES
48	a	486.59	7.70917	YES	YES
49	a	495.03	1.45340	YES	YES
50	a	507.34	4.79824	YES	YES

2fa

SCF Energy (au) BP86/SV(P)	-2391.961394095
SCF Energy (au) PBE0/def2-TZVPP	-2391.518095263
SCF Energy (au) PBE0/def2-TZVPP	-2391.5259797091 (Toluene Correction)
Zero Point Energy (au)	0.3211004
Chemical Potential (kJ mol^{-1})	689.84
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06699866

xyz coordinates
45

Mn	1.4798866	-0.2187247	0.6042757
C	1.9858282	0.1850369	2.2864095
C	3.1078742	-0.8153644	0.1948714
C	1.9261647	1.4494384	0.0171510
O	2.3355042	2.4877551	-0.3203568
O	4.1697173	-1.2232451	-0.0717724
O	2.3152063	0.4401459	3.3737385
C	-1.1801954	-0.8102208	1.8566652
C	-1.2646296	1.3042492	0.8362574
C	-2.6149049	1.4850452	1.2047053
C	-3.2443526	0.4625696	1.9267944
C	-2.5298906	-0.6901692	2.2573493
C	-0.3367492	-1.9750680	2.1535723
C	1.0015422	-1.9308193	1.6664095
C	1.8409481	-3.0288489	1.9547913
C	1.3735263	-4.1396970	2.6779099
C	0.0448376	-4.1782901	3.1430338
C	-0.8044324	-3.0978098	2.8820827
O	-0.5611747	2.2223023	0.1479445
H	-3.1579348	2.4008478	0.9352112
H	-4.2982282	0.5728714	2.2309414
H	-3.0099922	-1.4987815	2.8248023
H	2.8878098	-3.0300007	1.6082221
H	2.0544672	-4.9834827	2.8831749
H	-0.3244333	-5.0473483	3.7115733
H	-1.8414812	-3.1328419	3.2538322
N	-0.5632583	0.1880328	1.1483020
C	0.5092592	0.5040600	-2.6026110
C	1.5628757	1.2155775	-3.2293841
C	1.3059008	2.0406282	-4.3338314
C	-0.0025131	2.1825144	-4.8298025
C	-1.0570294	1.4841539	-4.2145901
C	-0.8076042	0.6527288	-3.1127119
H	2.5900246	1.1076915	-2.8487855
H	2.1398662	2.5794532	-4.8133716
H	-0.1994433	2.8342939	-5.6969663
H	-2.0855771	1.5825957	-4.6007656
H	-1.6311973	0.0979856	-2.6352136
C	0.7397492	-0.3979229	-1.4957523
C	0.6903825	-1.4982035	-0.8680577
H	0.5017714	-2.5721248	-0.8433323
C	-1.1618881	3.4526384	-0.2331367
H	-0.3662870	4.0176456	-0.7566458
H	-1.5042302	4.0308366	0.6560919
H	-2.0157150	3.2878659	-0.9290253

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.69	0.21459	YES	YES
8	a	29.61	0.05641	YES	YES
9	a	34.01	0.12405	YES	YES
10	a	43.43	0.08971	YES	YES
11	a	63.13	1.35943	YES	YES
12	a	75.59	1.13964	YES	YES
13	a	80.60	0.41255	YES	YES
14	a	90.18	0.49284	YES	YES
15	a	93.53	0.02787	YES	YES
16	a	100.58	0.83466	YES	YES
17	a	114.14	0.30028	YES	YES
18	a	118.32	0.18218	YES	YES
19	a	122.21	0.39617	YES	YES
20	a	129.25	0.90286	YES	YES
21	a	154.99	1.38789	YES	YES
22	a	156.86	0.72739	YES	YES
23	a	167.85	3.83857	YES	YES
24	a	182.29	1.19717	YES	YES
25	a	218.81	0.80044	YES	YES
26	a	229.75	0.95873	YES	YES
27	a	242.21	3.23163	YES	YES
28	a	254.84	0.06903	YES	YES
29	a	288.66	0.56483	YES	YES
30	a	305.04	0.17203	YES	YES
31	a	324.49	21.26696	YES	YES
32	a	334.75	2.71008	YES	YES
33	a	402.42	0.01934	YES	YES
34	a	407.91	0.84390	YES	YES
35	a	415.07	4.41464	YES	YES
36	a	435.04	8.05753	YES	YES
37	a	454.51	15.75093	YES	YES
38	a	459.11	2.46109	YES	YES
39	a	471.16	4.40160	YES	YES
40	a	478.30	3.94107	YES	YES
41	a	490.99	6.31778	YES	YES
42	a	499.39	3.20063	YES	YES
43	a	508.02	18.13741	YES	YES
44	a	513.95	2.54387	YES	YES
45	a	529.00	31.57498	YES	YES
46	a	536.56	11.31513	YES	YES
47	a	541.47	12.12873	YES	YES
48	a	555.01	2.26347	YES	YES
49	a	581.31	2.25487	YES	YES
50	a	606.94	24.76174	YES	YES

2ej

SCF Energy (au) BP86/SV(P)	-2814.654527730
SCF Energy (au) PBE0/def2-TZVPP	-2814.168815490
SCF Energy (au) PBE0/def2-TZVPP	-2814.1792225655 (Toluene Correction)
Zero Point Energy (au)	0.4650797
Chemical Potential (kJ mol^{-1})	1029.53
Dispersion Correction (au) PBE0/def2-TZVPP	-0.09205668

xyz coordinates
63

Mn	1.9456160	1.1548608	0.1958505
C	2.3174964	1.7535376	1.8490724
C	3.6459403	0.6209492	-0.0252364
C	2.2417920	2.8057008	-0.5079093
O	2.4490777	3.8871159	-0.8928812
O	4.7469566	0.2515105	-0.1584022
O	2.5659906	2.1407198	2.9191820
C	-0.7687233	0.6675232	1.1429281
C	-2.2330554	0.8694433	1.2963279
C	-0.0099007	-0.4218190	1.7424040
C	1.3817626	-0.4320683	1.4019474
C	2.1968402	-1.4323580	1.9608592
C	1.6568351	-2.4100915	2.8285623
C	0.2808277	-2.3773202	3.1737144
C	-0.5390031	-1.3877409	2.6386067
H	3.2693013	-1.4571753	1.7161129
O	2.3758798	-3.4141733	3.3952372
H	-0.1049106	-3.1348798	3.8732171
H	-1.6006016	-1.3485107	2.9327252
N	-0.0394002	1.5042181	0.4342321
C	0.7799226	1.6009485	-2.9389564
C	1.6257514	2.4310501	-3.7179503
C	1.0916549	3.2341651	-4.7350415
C	-0.2917779	3.2368847	-4.9889727
C	-1.1411542	2.4223127	-4.2198555
C	-0.6147849	1.6105739	-3.2041981
H	2.7091332	2.4347565	-3.5215034
H	1.7642898	3.8688724	-5.3354938
H	-0.7074816	3.8743582	-5.7867409
H	-2.2266108	2.4146907	-4.4148064
H	-1.2773778	0.9640588	-2.6069194
C	1.3055038	0.7353344	-1.9069689
C	1.5375929	-0.3836632	-1.3569005
C	1.7895150	-1.8090780	-1.4301288
C	-5.0344965	1.3238325	1.5025429
C	-4.5355261	0.0372441	1.1888465
C	-3.1605106	-0.1846951	1.0941285
C	-2.7457344	2.1499997	1.6003473
C	-4.1252938	2.3847820	1.7093693
O	-6.3870314	1.4358920	1.5812182
H	-5.2583003	-0.7757992	1.0176185
H	-2.7951668	-1.1888858	0.8259732
H	-2.0473340	2.9833999	1.7849273
H	-4.4783142	3.3945124	1.9645007
H	-0.5664635	2.2572249	-0.0305651
C	-6.9544541	2.7007651	1.8840578
H	-6.6311035	3.0681702	2.8864834
H	-8.0526205	2.5505129	1.8903394
H	-6.6950736	3.4643635	1.1130867
C	3.7623117	-3.5203748	3.1025461
H	4.3241281	-2.6193473	3.4428990
H	3.9408832	-3.6724222	2.0130853

```
H     4.1242530   -4.4071241    3.6610765
C     2.2998198   -4.5825249   -1.6992044
C     1.1606521   -4.1354233   -1.0061845
C     0.9082016   -2.7631267   -0.8644706
C     2.9391798   -2.2701009   -2.1219546
C     3.1886010   -3.6441445   -2.2533474
H     2.4955186   -5.6624250   -1.8064831
H     0.4604443   -4.8642520   -0.5655675
H     0.0205352   -2.4157940   -0.3143619
H     3.6347926   -1.5346342   -2.5551036
H     4.0852046   -3.9843320   -2.7979179

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              11.41         0.09327       YES     YES
     8        a              16.85         0.05804       YES     YES
     9        a              20.99         0.16957       YES     YES
    10        a              28.16         0.10066       YES     YES
    11        a              36.00         0.86956       YES     YES
    12        a              39.01         0.31055       YES     YES
    13        a              45.19         0.10445       YES     YES
    14        a              48.27         0.84812       YES     YES
    15        a              53.24         0.12915       YES     YES
    16        a              61.97         0.17545       YES     YES
    17        a              70.80         0.30147       YES     YES
    18        a              77.93         0.10995       YES     YES
    19        a              83.73         0.90023       YES     YES
    20        a              90.22         0.23146       YES     YES
    21        a              94.80         0.17699       YES     YES
    22        a              98.30         0.47627       YES     YES
    23        a             104.33         0.89218       YES     YES
    24        a             109.49         0.93333       YES     YES
    25        a             118.15         1.82754       YES     YES
    26        a             146.42         1.64226       YES     YES
    27        a             150.95         1.34614       YES     YES
    28        a             158.67         0.88868       YES     YES
    29        a             169.35         2.88200       YES     YES
    30        a             181.04         2.40710       YES     YES
    31        a             188.68         3.26368       YES     YES
    32        a             191.67         1.53467       YES     YES
    33        a             206.86         0.62635       YES     YES
    34        a             230.76         3.27932       YES     YES
    35        a             234.86         2.02230       YES     YES
    36        a             248.55         0.36116       YES     YES
    37        a             253.94         1.23472       YES     YES
    38        a             267.87         0.75825       YES     YES
    39        a             296.61         3.74998       YES     YES
    40        a             320.41         2.34102       YES     YES
    41        a             341.10         0.88454       YES     YES
    42        a             360.93         5.44085       YES     YES
    43        a             376.09        10.14822       YES     YES
    44        a             382.42        32.74494       YES     YES
    45        a             401.20         0.01273       YES     YES
    46        a             402.61         0.11511       YES     YES
    47        a             415.93         2.26611       YES     YES
    48        a             421.73         1.09351       YES     YES
```

49	a	440.76	4.23288	YES	YES
50	a	453.33	1.25458	YES	YES

2fa'

SCF Energy (au) BP86/SV(P) -2391.959491985
SCF Energy (au) PBE0/def2-TZVPP -2391.516131723
SCF Energy (au) PBE0/def2-TZVPP -2391.5242788848 (Toluene Correction)
Zero Point Energy (au) 0.3212083
Chemical Potential (kJ mol^{-1}) 690.67
Dispersion Correction (au) PBE0/def2-TZVPP -0.06847143

xyz coordinates
45

Mn	1.3963769	1.3583796	0.3444836
C	1.4957594	1.7909642	2.0933701
C	3.1423484	1.0164151	0.2487564
C	1.6670801	3.0927734	-0.1289336
O	1.9417192	4.1914285	-0.4091898
O	4.2810258	0.7630211	0.1844692
O	1.5645760	2.0826934	3.2182820
C	-1.3013999	0.2766545	1.0687616
C	-1.5652880	2.3506976	-0.0038004
C	-2.9709816	2.2805102	0.0915204
C	-3.5348398	1.1533677	0.7050525
C	-2.7031045	0.1460634	1.1961401
C	-0.3361981	-0.7167661	1.5532949
C	1.0401974	-0.4292863	1.3235092
C	1.9895755	-1.3493861	1.8180369
C	1.5987860	-2.5251865	2.4814980
C	0.2347955	-2.8085505	2.6814675
C	-0.7272833	-1.9041925	2.2201260
O	-0.9183472	3.3876342	-0.5742201
H	-3.6082712	3.0827651	-0.3038207
H	-4.6300732	1.0672355	0.7956806
H	-3.1312896	-0.7437030	1.6772621
H	3.0676964	-1.1558228	1.6898941
H	2.3676865	-3.2262140	2.8491260
H	-0.0759951	-3.7294558	3.2012154
H	-1.7934148	-2.1283994	2.3874980
N	-0.7487716	1.3797544	0.4702178
H	1.2478329	2.1441806	-2.5348533
C	1.1781634	1.3641921	-1.7754152
C	1.0614090	0.1419872	-1.4550057
C	0.8178416	-1.2600164	-1.7094089
C	0.3304515	-3.9864540	-2.2994260
C	1.5879058	-3.5794731	-1.8181482
C	1.8312532	-2.2322700	-1.5175448
C	-0.4470777	-1.6804654	-2.1938190
C	-0.6847403	-3.0319935	-2.4845658
H	0.1423019	-5.0482405	-2.5298388
H	2.3899640	-4.3218948	-1.6721158
H	2.8161788	-1.9143457	-1.1427412
H	-1.2399391	-0.9305886	-2.3445678
H	-1.6733543	-3.3420701	-2.8625993
C	-1.6486398	4.5142629	-1.0398888
H	-2.3272451	4.2424261	-1.8811164
H	-0.8856423	5.2328984	-1.3984561
H	-2.2390287	4.9844696	-0.2201868

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.56	0.32176	YES	YES
8	a	30.56	0.34957	YES	YES
9	a	35.61	0.34595	YES	YES
10	a	46.86	0.06387	YES	YES
11	a	53.70	0.06745	YES	YES
12	a	73.53	1.80693	YES	YES
13	a	80.07	0.76770	YES	YES
14	a	92.33	0.60385	YES	YES
15	a	96.13	0.24797	YES	YES
16	a	101.05	0.13766	YES	YES
17	a	109.72	0.88510	YES	YES
18	a	118.53	0.25899	YES	YES
19	a	120.29	0.21308	YES	YES
20	a	126.82	0.65942	YES	YES
21	a	156.16	0.25574	YES	YES
22	a	164.73	0.43699	YES	YES
23	a	176.58	2.86296	YES	YES
24	a	184.23	1.52408	YES	YES
25	a	219.10	0.21957	YES	YES
26	a	232.13	1.09117	YES	YES
27	a	233.24	1.55831	YES	YES
28	a	263.08	0.18058	YES	YES
29	a	289.97	0.69181	YES	YES
30	a	308.04	0.41727	YES	YES
31	a	325.07	11.81392	YES	YES
32	a	334.42	1.62532	YES	YES
33	a	400.32	0.77081	YES	YES
34	a	407.09	10.83810	YES	YES
35	a	409.88	5.26984	YES	YES
36	a	430.73	0.31742	YES	YES
37	a	458.21	1.77025	YES	YES
38	a	461.90	4.09505	YES	YES
39	a	472.38	4.53511	YES	YES
40	a	482.55	7.02191	YES	YES
41	a	493.96	3.82026	YES	YES
42	a	498.09	3.42824	YES	YES
43	a	506.42	21.10995	YES	YES
44	a	508.51	0.81419	YES	YES
45	a	529.26	8.32951	YES	YES
46	a	537.81	17.08554	YES	YES
47	a	541.32	2.62297	YES	YES
48	a	568.59	3.32784	YES	YES
49	a	581.32	2.91337	YES	YES
50	a	612.10	26.50879	YES	YES

2ga

SCF Energy (au) BP86/SV(P) -2508.397058357
SCF Energy (au) PBE0/def2-TZVPP -2507.918314687
SCF Energy (au) PBE0/def2-TZVPP -2507.9263616631 (Toluene Correction)
Zero Point Energy (au) 0.3679099
Chemical Potential (kJ mol^{-1}) 804.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.08238683

xyz coordinates
51

Mn	1.4627019	-0.6136569	0.6719518
C	1.9354949	0.0695481	2.2687287
C	3.0921388	-1.2780301	0.4018875
C	1.9643077	0.8904391	-0.2341898
O	2.4492548	1.7919919	-0.7928015
O	4.1559398	-1.7320077	0.2404221
O	2.2409436	0.4997903	3.3074133
C	-1.2743036	-1.2048065	1.6578451
C	-1.3235574	0.9260137	0.6467378
C	-2.7339246	0.9150606	0.6335650
C	-3.4234327	-0.1952212	1.1390735
C	-2.6868249	-1.2467250	1.6858767
C	-0.4209420	-2.2522340	2.2349893
C	0.9717282	-2.1633040	1.9506955
C	1.8238570	-3.1294950	2.5254005
C	1.3197737	-4.1548839	3.3444704
C	-0.0604725	-4.2411538	3.6088029
C	-0.9265764	-3.2923808	3.0539203
C	-0.6419949	2.2018926	0.2795213
H	-3.2694568	1.8023754	0.2637775
H	-4.5254493	-0.2231023	1.1354352
H	-3.1980078	-2.1159172	2.1239789
H	2.9098132	-3.0934209	2.3361770
H	2.0124835	-4.8924719	3.7849519
H	-0.4575073	-5.0421799	4.2535378
H	-2.0039605	-3.3563542	3.2794642
N	-0.6094863	-0.1505738	1.0806026
C	0.3156615	-0.4401438	-2.5752413
C	1.2673483	0.2390870	-3.3774685
C	0.8691893	0.8875930	-4.5549764
C	-0.4793001	0.8783310	-4.9545738
C	-1.4323542	0.2068282	-4.1678224
C	-1.0430860	-0.4459915	-2.9889960
H	2.3248815	0.2482745	-3.0744248
H	1.6234532	1.4069923	-5.1688521
H	-0.7868842	1.3911799	-5.8809002
H	-2.4908057	0.1869449	-4.4772127
H	-1.7867481	-0.9773241	-2.3740579
C	0.6874200	-1.1659350	-1.3824163
C	0.7767075	-2.1594344	-0.6038190
H	0.7188242	-3.2323749	-0.4197090
C	0.4681783	4.7342046	-0.2978530
C	0.6605090	4.1523752	0.9671899
C	0.1111930	2.8946908	1.2554809
C	-0.8466833	2.8017314	-0.9816079
C	-0.2847516	4.0553750	-1.2705521
H	0.9067758	5.7197436	-0.5261296
H	1.2440403	4.6821833	1.7380140
H	0.2553213	2.4465547	2.2516542
H	-1.4278246	2.2673028	-1.7507523
H	-0.4336055	4.5026188	-2.2672091

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.36	0.19938	YES	YES
8	a	27.51	0.04880	YES	YES
9	a	38.08	0.05465	YES	YES
10	a	42.39	0.27325	YES	YES
11	a	57.15	0.17486	YES	YES
12	a	68.93	0.12536	YES	YES
13	a	74.12	0.12993	YES	YES
14	a	75.27	0.85869	YES	YES
15	a	81.84	0.06469	YES	YES
16	a	89.05	0.58480	YES	YES
17	a	93.51	0.42378	YES	YES
18	a	111.22	0.16990	YES	YES
19	a	113.13	0.03525	YES	YES
20	a	117.12	0.61225	YES	YES
21	a	121.99	0.37536	YES	YES
22	a	139.20	0.58041	YES	YES
23	a	155.50	4.72657	YES	YES
24	a	160.00	0.76063	YES	YES
25	a	175.36	1.07927	YES	YES
26	a	210.04	0.69555	YES	YES
27	a	220.26	0.16892	YES	YES
28	a	237.95	1.93218	YES	YES
29	a	242.94	2.19533	YES	YES
30	a	294.11	2.09996	YES	YES
31	a	314.01	0.68797	YES	YES
32	a	321.10	19.21421	YES	YES
33	a	337.85	1.48906	YES	YES
34	a	372.54	1.02664	YES	YES
35	a	400.01	0.24974	YES	YES
36	a	401.56	0.02427	YES	YES
37	a	410.61	5.14172	YES	YES
38	a	431.09	4.52154	YES	YES
39	a	450.68	15.38779	YES	YES
40	a	459.24	1.28575	YES	YES
41	a	465.75	4.47669	YES	YES
42	a	476.92	5.61536	YES	YES
43	a	477.59	5.69098	YES	YES
44	a	489.88	4.79517	YES	YES
45	a	498.86	8.36890	YES	YES
46	a	505.49	15.89184	YES	YES
47	a	512.07	0.41507	YES	YES
48	a	525.04	22.93634	YES	YES
49	a	539.12	9.81531	YES	YES
50	a	545.76	4.36875	YES	YES

2ga'

SCF Energy (au) BP86/SV(P)		-2508.396040454
SCF Energy (au) PBE0/def2-TZVPP		-2507.916677625
SCF Energy (au) PBE0/def2-TZVPP		-2507.9248487015 (Toluene Correction)
Zero Point Energy (au)		0.3677349
Chemical Potential (kJ mol^{-1})		803.07
Dispersion Correction (au)	PBE0/def2-TZVPP	-0.08281505

xyz coordinates
51

Mn	1.4391057	0.6238850	0.2962395
C	1.6057090	1.2800530	1.9682203
C	3.1384581	0.0991255	0.2177723
C	1.9242572	2.2136855	-0.4425164
O	2.3853360	3.1769319	-0.9117753
O	4.2454900	-0.2706716	0.1786023
O	1.7088666	1.7165425	3.0427783
C	-1.3073847	-0.3107272	0.9690128
C	-1.5041005	1.7935720	-0.0768454
C	-2.8934610	1.6153724	-0.2371849
C	-3.4956725	0.4332819	0.2151002
C	-2.6999867	-0.5227177	0.8463202
C	-0.4005191	-1.2565522	1.6317917
C	0.9936664	-1.0095990	1.4871117
C	1.8834806	-1.8698532	2.1640286
C	1.4185878	-2.9515258	2.9324487
C	0.0385806	-3.1996671	3.0476429
C	-0.8663112	-2.3526857	2.3985808
C	-0.9366685	3.1277568	-0.4318752
H	-3.4886153	2.4275855	-0.6811821
H	-4.5799235	0.2729178	0.0967109
H	-3.1447986	-1.4512244	1.2310743
H	2.9721522	-1.7048341	2.1004869
H	2.1417944	-3.6047800	3.4502864
H	-0.3304881	-4.0452930	3.6506908
H	-1.9468188	-2.5412764	2.5099494
N	-0.7183081	0.8205497	0.4609888
H	1.1918898	1.0978682	-2.6496469
C	1.1094174	0.4155304	-1.8019133
C	0.9619543	-0.7563221	-1.3339748
C	0.6429493	-2.1626103	-1.4536003
C	0.0072647	-4.9014407	-1.7918630
C	1.2330252	-4.5245521	-1.2139585
C	1.5483836	-3.1703207	-1.0374688
C	-0.5901544	-2.5528379	-2.0368187
C	-0.9018073	-3.9104278	-2.2019866
H	-0.2391899	-5.9682252	-1.9226733
H	1.9521015	-5.2959201	-0.8921393
H	2.5079090	-2.8774387	-0.5853995
H	-1.2990600	-1.7747098	-2.3615368
H	-1.8639889	-4.1971431	-2.6585568
C	-0.0654151	5.7462825	-1.0362026
C	0.0314850	5.2560744	0.2776686
C	-0.3981314	3.9555611	0.5794579
C	-1.0496012	3.6351764	-1.7444527
C	-0.6052271	4.9326472	-2.0465734
H	0.2807037	6.7657957	-1.2734075
H	0.4487774	5.8915806	1.0758772
H	-0.3250503	3.5756515	1.6111820
H	-1.4787104	2.9993103	-2.5369369
H	-0.6819526	5.3106181	-3.0795345

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.68	0.02458	YES	YES
8	a	20.00	0.02170	YES	YES
9	a	26.94	0.27393	YES	YES
10	a	44.89	0.09041	YES	YES
11	a	52.65	0.10546	YES	YES
12	a	55.18	0.14935	YES	YES
13	a	68.98	0.10168	YES	YES
14	a	75.19	0.90378	YES	YES
15	a	80.23	0.43735	YES	YES
16	a	95.98	0.04786	YES	YES
17	a	96.61	0.15507	YES	YES
18	a	105.08	0.15543	YES	YES
19	a	111.34	0.29671	YES	YES
20	a	118.14	0.38801	YES	YES
21	a	124.61	0.95451	YES	YES
22	a	137.24	0.09103	YES	YES
23	a	158.46	0.86799	YES	YES
24	a	174.47	1.38164	YES	YES
25	a	183.09	1.57158	YES	YES
26	a	200.25	0.43881	YES	YES
27	a	216.64	0.84383	YES	YES
28	a	229.46	1.29740	YES	YES
29	a	240.10	0.08552	YES	YES
30	a	297.63	0.15925	YES	YES
31	a	311.68	0.62241	YES	YES
32	a	330.86	11.24064	YES	YES
33	a	337.66	1.74335	YES	YES
34	a	370.52	1.39688	YES	YES
35	a	399.39	0.24768	YES	YES
36	a	399.93	0.79518	YES	YES
37	a	407.82	14.42548	YES	YES
38	a	426.95	0.94010	YES	YES
39	a	453.00	0.03982	YES	YES
40	a	459.14	3.39036	YES	YES
41	a	462.50	8.72856	YES	YES
42	a	476.80	6.22106	YES	YES
43	a	481.75	0.17525	YES	YES
44	a	490.98	5.09356	YES	YES
45	a	499.22	0.51778	YES	YES
46	a	505.01	18.43589	YES	YES
47	a	512.38	4.66827	YES	YES
48	a	531.55	4.58873	YES	YES
49	a	541.02	12.91639	YES	YES
50	a	549.53	3.33764	YES	YES

2ha

SCF Energy (au) BP86/SV(P) -2354.867702753
SCF Energy (au) PBE0/def2-TZVPP -2354.415337120
SCF Energy (au) PBE0/def2-TZVPP -2354.4233622997 (Toluene Correction)
Zero Point Energy (au) 0.3227920
Chemical Potential (kJ mol^{-1}) 692.09
Dispersion Correction (au) PBE0/def2-TZVPP -0.06448300

xyz coordinates
45

Mn	1.9844632	0.3615964	0.2805713
C	2.4729053	0.7706078	1.9633091
C	3.6802028	-0.0913158	-0.1161913
C	2.1691997	2.0841028	-0.2778616
O	2.2954408	3.2028442	-0.5801308
O	4.7776609	-0.3989431	-0.3667064
O	2.7934382	1.0254737	3.0533302
C	-0.6474250	-0.2993731	1.3472536
C	-2.0987172	-0.1416954	1.6399885
C	0.1625301	-1.4533976	1.7369729
C	1.5284218	-1.3774515	1.3141167
C	2.3774492	-2.4442437	1.6743531
C	1.8981386	-3.5411240	2.4143880
C	0.5545604	-3.5942075	2.8362105
C	-0.3123366	-2.5468645	2.5030714
H	3.4404841	-2.4287957	1.3790219
H	2.5876445	-4.3616677	2.6781061
H	0.1908380	-4.4464731	3.4329670
H	-1.3580410	-2.5659727	2.8511029
N	0.0191421	0.6347120	0.7090967
C	0.9878452	1.0097481	-2.9360200
C	1.9878718	1.7884232	-3.5718213
C	1.6561809	2.6351458	-4.6380820
C	0.3254007	2.7326849	-5.0831244
C	-0.6758427	1.9707337	-4.4556397
C	-0.3522845	1.1163009	-3.3916256
H	3.0304467	1.7157479	-3.2248581
H	2.4468762	3.2286812	-5.1259904
H	0.0691267	3.4043029	-5.9190083
H	-1.7212712	2.0399266	-4.7997030
H	-1.1341259	0.5134927	-2.9024547
C	1.3062087	0.0918749	-1.8676401
C	1.4093925	-1.0031709	-1.2426333
H	1.3803549	-2.0928587	-1.2210400
C	-4.8598289	0.2380123	2.1238249
C	-4.4023850	-0.9573970	1.5420035
C	-3.0322054	-1.1508820	1.3058817
C	-2.5709113	1.0600181	2.2188912
C	-3.9402320	1.2457316	2.4628171
H	-5.9358974	0.3841697	2.3141531
H	-5.1204428	-1.7467476	1.2648043
H	-2.6820451	-2.0814766	0.8311990
H	-1.8499617	1.8443132	2.5038226
H	-4.2907055	2.1823146	2.9268384
H	-0.5475650	1.4430989	0.4124348

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.29	0.15192	YES	YES
8	a	23.03	0.07633	YES	YES
9	a	33.10	0.10247	YES	YES
10	a	43.98	0.05862	YES	YES
11	a	51.74	0.15394	YES	YES
12	a	61.36	0.17907	YES	YES
13	a	71.43	0.28741	YES	YES
14	a	78.72	0.06019	YES	YES
15	a	85.78	0.82130	YES	YES
16	a	91.19	0.05240	YES	YES
17	a	99.69	0.24511	YES	YES
18	a	109.24	0.33295	YES	YES
19	a	115.10	0.66219	YES	YES
20	a	126.70	0.21360	YES	YES
21	a	150.72	0.94188	YES	YES
22	a	160.87	5.74710	YES	YES
23	a	185.99	0.60228	YES	YES
24	a	204.17	1.78023	YES	YES
25	a	214.52	2.04916	YES	YES
26	a	236.75	1.95956	YES	YES
27	a	274.26	2.42220	YES	YES
28	a	308.38	1.57647	YES	YES
29	a	317.62	23.99863	YES	YES
30	a	353.85	0.52186	YES	YES
31	a	399.49	0.02689	YES	YES
32	a	403.76	0.21821	YES	YES
33	a	410.32	4.31237	YES	YES
34	a	421.74	6.72909	YES	YES
35	a	446.90	9.46617	YES	YES
36	a	451.86	1.39235	YES	YES
37	a	464.55	11.74879	YES	YES
38	a	477.59	6.21398	YES	YES
39	a	488.60	4.57895	YES	YES
40	a	490.74	0.53493	YES	YES
41	a	495.96	12.78844	YES	YES
42	a	501.78	3.93526	YES	YES
43	a	503.02	13.71281	YES	YES
44	a	524.14	33.20199	YES	YES
45	a	536.84	10.50917	YES	YES
46	a	546.50	11.89717	YES	YES
47	a	584.32	10.55322	YES	YES
48	a	609.23	6.23246	YES	YES
49	a	611.60	6.04316	YES	YES
50	a	618.08	26.29849	YES	YES

2ha'

SCF Energy (au) BP86/SV(P) -2354.864921936
SCF Energy (au) PBE0/def2-TZVPP -2354.412686755
SCF Energy (au) PBE0/def2-TZVPP -2354.4205956618 (Toluene Correction)
Zero Point Energy (au) 0.3226891
Chemical Potential (kJ mol^{-1}) 689.13
Dispersion Correction (au) PBE0/def2-TZVPP -0.06741741

xyz coordinates
45

Mn	1.7370355	1.9156621	-0.0185669
C	1.9577555	2.3012045	1.7280394
C	3.5025465	1.6204490	-0.1985573
C	1.8152550	3.6694973	-0.4796261
O	1.8576291	4.8024604	-0.7541614
O	4.6427294	1.3986452	-0.3138999
O	2.1139695	2.5589014	2.8526198
C	-0.9128298	0.9532138	0.7371207
C	-0.0320248	-0.1264507	1.1817887
C	1.3579263	0.1145890	0.9381381
C	2.2687341	-0.8681919	1.3733419
C	1.8252121	-2.0586472	1.9791169
C	0.4511831	-2.3013110	2.1698957
C	-0.4790054	-1.3349730	1.7693790
H	3.3531148	-0.7201772	1.2347946
H	2.5643202	-2.8133496	2.2986332
H	0.1092259	-3.2436898	2.6277984
H	-1.5577047	-1.5208744	1.8999189
N	-0.2877921	1.9497253	0.1541413
H	1.4157086	2.6883447	-2.9025956
C	1.4505005	1.8998432	-2.1490172
C	1.4570271	0.6712439	-1.8394499
C	1.3933284	-0.7536490	-2.0724049
C	1.2754370	-3.5277641	-2.6245405
C	2.5071684	-2.9174475	-2.3265894
C	2.5693084	-1.5455561	-2.0451657
C	0.1564402	-1.3787876	-2.3703728
C	0.1022075	-2.7536656	-2.6432421
H	1.2301733	-4.6077036	-2.8416829
H	3.4320346	-3.5175530	-2.3114330
H	3.5339045	-1.0675370	-1.8131480
H	-0.7618670	-0.7708876	-2.3936988
H	-0.8675413	-3.2241721	-2.8760245
C	-2.3914229	0.9752072	0.9151925
C	-5.1970723	1.1358492	1.2411788
C	-4.3749026	0.8234653	2.3378931
C	-2.9827916	0.7378493	2.1781861
C	-3.2278479	1.2961468	-0.1798602
C	-4.6198514	1.3707898	-0.0187747
H	-6.2904248	1.1971927	1.3691612
H	-4.8210463	0.6497995	3.3310303
H	-2.3425002	0.5151240	3.0466631
H	-2.7787729	1.4666498	-1.1727490
H	-5.2587493	1.6098494	-0.8848484
H	-0.8957280	2.7306852	-0.1336224

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.23	0.02192	YES	YES
8	a	16.44	0.10699	YES	YES
9	a	38.20	0.10104	YES	YES
10	a	42.72	0.17829	YES	YES
11	a	54.28	0.13952	YES	YES
12	a	54.98	0.02477	YES	YES
13	a	69.67	0.51001	YES	YES
14	a	79.26	0.02376	YES	YES
15	a	85.42	0.70115	YES	YES
16	a	94.94	0.21828	YES	YES
17	a	99.78	0.07365	YES	YES
18	a	104.02	0.58385	YES	YES
19	a	112.90	0.20273	YES	YES
20	a	127.26	0.35518	YES	YES
21	a	157.98	1.20516	YES	YES
22	a	169.08	0.84161	YES	YES
23	a	175.46	2.55549	YES	YES
24	a	203.10	0.94757	YES	YES
25	a	216.55	1.45099	YES	YES
26	a	229.83	0.29463	YES	YES
27	a	272.63	3.00912	YES	YES
28	a	305.65	0.53639	YES	YES
29	a	312.82	13.43462	YES	YES
30	a	353.75	0.62675	YES	YES
31	a	397.88	2.80142	YES	YES
32	a	400.74	9.57004	YES	YES
33	a	404.39	1.69232	YES	YES
34	a	419.99	0.68333	YES	YES
35	a	447.42	0.40847	YES	YES
36	a	455.05	2.94910	YES	YES
37	a	471.57	3.81417	YES	YES
38	a	482.56	9.46046	YES	YES
39	a	483.31	3.76855	YES	YES
40	a	490.41	6.60203	YES	YES
41	a	496.41	2.36391	YES	YES
42	a	499.52	17.06561	YES	YES
43	a	504.97	7.12513	YES	YES
44	a	520.67	15.02069	YES	YES
45	a	535.37	8.58747	YES	YES
46	a	560.04	8.32210	YES	YES
47	a	586.03	3.19765	YES	YES
48	a	610.13	0.63566	YES	YES
49	a	612.40	6.56616	YES	YES
50	a	619.97	64.61582	YES	YES

2ia

SCF Energy (au) BP86/SV(P) -2183.122606432
SCF Energy (au) PBE0/def2-TZVPP -2182.706625903
SCF Energy (au) PBE0/def2-TZVPP -2182.7132650811 (Toluene Correction)
Zero Point Energy (au) 0.2582288
Chemical Potential (kJ mol^{-1}) 536.57
Dispersion Correction (au) PBE0/def2-TZVPP -0.05063461

xyz coordinates
37

Mn	1.0276323	0.3512433	0.9392188
C	1.1370934	0.6341023	2.7177790
C	2.7601907	-0.0495923	0.8708951
C	1.3101813	2.1264881	0.5941055
O	1.5153634	3.2602778	0.4386312
O	3.8873994	-0.3513020	0.8262138
O	1.2212734	0.7993244	3.8667371
C	-1.7321304	-0.3567563	1.3365823
C	-3.2367423	-0.2400642	1.3456914
C	-1.0221630	-1.5557674	1.7671824
C	0.4036238	-1.4598931	1.6766759
C	1.1509095	-2.5788773	2.1038483
C	0.5148944	-3.7386671	2.5790587
C	-0.8932832	-3.8219904	2.6497290
C	-1.6626598	-2.7286071	2.2444057
H	2.2532812	-2.5552050	2.0663755
H	1.1268527	-4.5975959	2.9050630
H	-1.3780831	-4.7378682	3.0247820
H	-2.7632359	-2.7795799	2.2979940
O	-1.0463227	0.6258788	0.9473827
C	0.5587890	1.3296505	-2.2859772
C	1.3550578	1.2794408	-3.4595080
C	1.1786239	2.2285641	-4.4762772
C	0.2087685	3.2381839	-4.3436773
C	-0.5854823	3.2952924	-3.1842105
C	-0.4119255	2.3550292	-2.1598384
H	2.1150387	0.4882493	-3.5600353
H	1.8061901	2.1801339	-5.3817235
H	0.0737329	3.9844462	-5.1440526
H	-1.3470002	4.0851299	-3.0747019
H	-1.0301008	2.3943804	-1.2493785
C	0.7254424	0.3200752	-1.2659808
C	0.8311265	-0.8453558	-0.7786278
H	0.8181768	-1.9306874	-0.8852514
H	-3.5372666	0.7642561	0.9869631
H	-3.6380547	-0.3971449	2.3717041
H	-3.6951916	-1.0151920	0.6922219

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.87	0.42459	YES	YES
8	a	33.85	0.18411	YES	YES
9	a	46.95	0.12673	YES	YES
10	a	57.10	0.04978	YES	YES
11	a	67.42	0.90009	YES	YES

12	a	77.84	0.13583	YES	YES
13	a	88.20	0.66367	YES	YES
14	a	95.47	0.27775	YES	YES
15	a	106.01	0.31080	YES	YES
16	a	109.13	0.52012	YES	YES
17	a	117.66	0.08236	YES	YES
18	a	119.11	0.12682	YES	YES
19	a	132.46	0.08321	YES	YES
20	a	169.13	3.07848	YES	YES
21	a	170.62	1.97929	YES	YES
22	a	210.75	1.15734	YES	YES
23	a	222.46	1.43356	YES	YES
24	a	242.47	1.64021	YES	YES
25	a	254.89	0.37087	YES	YES
26	a	288.22	0.78470	YES	YES
27	a	325.61	19.55637	YES	YES
28	a	402.00	0.15435	YES	YES
29	a	405.50	0.34124	YES	YES
30	a	411.25	1.72472	YES	YES
31	a	418.63	4.36502	YES	YES
32	a	440.28	9.11232	YES	YES
33	a	459.61	9.70023	YES	YES
34	a	470.59	1.75045	YES	YES
35	a	477.20	2.96730	YES	YES
36	a	488.01	10.85217	YES	YES
37	a	495.04	2.33308	YES	YES
38	a	505.71	2.73942	YES	YES
39	a	519.54	19.67222	YES	YES
40	a	524.75	36.41111	YES	YES
41	a	536.80	13.03176	YES	YES
42	a	548.38	3.82310	YES	YES
43	a	600.77	14.13686	YES	YES
44	a	608.60	4.43846	YES	YES
45	a	610.84	39.97431	YES	YES
46	a	613.49	3.98419	YES	YES
47	a	633.19	2.48601	YES	YES
48	a	649.36	55.39115	YES	YES
49	a	661.00	16.37113	YES	YES
50	a	677.34	63.83913	YES	YES

2ia'

SCF Energy (au) BP86/SV(P) -2183.119255411
SCF Energy (au) PBE0/def2-TZVPP -2182.703507634
SCF Energy (au) PBE0/def2-TZVPP -2182.7102422094 (Toluene Correction)
Zero Point Energy (au) 0.2582085
Chemical Potential (kJ mol^{-1}) 535.77
Dispersion Correction (au) PBE0/def2-TZVPP -0.05302657

xyz coordinates
37

Mn	0.8983506	2.1448421	0.2688325
C	0.9141654	2.6039852	2.0158285
C	2.6524396	1.8402962	0.2910139
C	1.0410226	3.8978391	-0.2149611
O	1.1379995	5.0217186	-0.4998359
O	3.7932662	1.5904865	0.3081505
O	0.9364859	2.9056166	3.1391041
C	-1.8075626	1.2690843	0.7174211
C	-3.3169564	1.2705979	0.7003573
C	-1.0157638	0.1978747	1.3120318
C	0.3991048	0.3910100	1.2188449
C	1.2199172	-0.5869534	1.8179770
C	0.6658534	-1.7165200	2.4456782
C	-0.7312506	-1.9033912	2.5086360
C	-1.5737069	-0.9425776	1.9432115
H	2.3172948	-0.4767215	1.8023292
H	1.3356915	-2.4674974	2.8992107
H	-1.1522350	-2.7932599	3.0039253
H	-2.6680678	-1.0712190	1.9941553
O	-1.1936215	2.2423079	0.2064007
H	0.8117751	2.8996123	-2.6174311
C	0.7709592	2.1278030	-1.8471192
C	0.7261974	0.9043305	-1.5060129
C	0.5963222	-0.5095824	-1.7921790
H	-3.6832412	2.1744501	0.1742166
H	-3.7192499	1.2647297	1.7380287
H	-3.7087963	0.3619751	0.1922516
C	0.3439853	-3.2490311	-2.4608312
C	-0.6892896	-2.3484622	-2.7736553
C	-0.5671662	-0.9900332	-2.4453026
C	1.6281109	-1.4273549	-1.4744203
C	1.5025775	-2.7816281	-1.8145887
H	0.2475396	-4.3157889	-2.7222773
H	-1.5990167	-2.7059184	-3.2843124
H	-1.3704902	-0.2800854	-2.6988473
H	2.5380412	-1.0612958	-0.9746253
H	2.3193148	-3.4812396	-1.5712059

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.26	0.07232	YES	YES
8	a	27.27	0.39170	YES	YES
9	a	49.44	0.19270	YES	YES
10	a	59.02	0.06082	YES	YES
11	a	63.52	0.04027	YES	YES

12	a	73.78	1.26466	YES	YES
13	a	88.99	0.65309	YES	YES
14	a	97.88	0.16892	YES	YES
15	a	104.69	0.28633	YES	YES
16	a	115.69	0.22641	YES	YES
17	a	117.80	0.85020	YES	YES
18	a	127.98	0.10742	YES	YES
19	a	131.86	0.42863	YES	YES
20	a	165.40	1.61920	YES	YES
21	a	182.02	1.60815	YES	YES
22	a	201.91	0.59779	YES	YES
23	a	222.49	1.74088	YES	YES
24	a	231.59	1.17169	YES	YES
25	a	254.48	0.63146	YES	YES
26	a	291.18	0.61839	YES	YES
27	a	328.62	12.16511	YES	YES
28	a	400.08	0.31887	YES	YES
29	a	406.66	6.49271	YES	YES
30	a	409.60	3.66119	YES	YES
31	a	416.98	3.55152	YES	YES
32	a	450.74	2.33025	YES	YES
33	a	460.02	1.33503	YES	YES
34	a	470.60	3.95403	YES	YES
35	a	478.52	6.71100	YES	YES
36	a	492.43	11.27503	YES	YES
37	a	497.15	3.54688	YES	YES
38	a	502.61	9.37704	YES	YES
39	a	511.36	10.56242	YES	YES
40	a	526.42	16.87395	YES	YES
41	a	535.87	6.33441	YES	YES
42	a	566.15	5.67608	YES	YES
43	a	601.71	15.77670	YES	YES
44	a	608.29	5.91649	YES	YES
45	a	612.50	14.51577	YES	YES
46	a	616.09	56.93462	YES	YES
47	a	633.33	2.95790	YES	YES
48	a	647.28	41.26479	YES	YES
49	a	652.92	19.21428	YES	YES
50	a	679.40	77.09036	YES	YES

2ja

SCF Energy (au) BP86/SV(P)	-2452.080768239
SCF Energy (au) PBE0/def2-TZVPP	-2451.620892726
SCF Energy (au) PBE0/def2-TZVPP	-2451.6286920118 (Toluene Correction)
Zero Point Energy (au)	0.3431713
Chemical Potential (kJ mol^{-1})	738.84
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06762876

xyz coordinates
48

Mn	1.3428078	0.8045502	0.5807547
C	1.3783701	1.2227344	2.3336199
C	3.1025940	0.4977164	0.5670520
C	1.5688369	2.5632149	0.1210029
O	1.7224449	3.6913483	-0.1112692
O	4.2521930	0.2995053	0.5355771
O	1.4098099	1.4889051	3.4667047
C	-1.3953526	0.0611476	0.8785204
C	-2.8797304	0.1605952	0.8509716
C	-0.6783374	-1.0867017	1.3610949
C	0.7053038	-0.9939985	1.3398313
C	1.5223928	-2.1348688	1.7934017
O	-0.7101442	1.0584446	0.4739061
C	0.9310357	1.5353758	-2.7143732
C	1.7985379	1.5006747	-3.8368380
C	1.6046139	2.3843498	-4.9078489
C	0.5482648	3.3121502	-4.8796436
C	-0.3155739	3.3537136	-3.7703583
C	-0.1271098	2.4784202	-2.6927061
H	2.6264471	0.7741179	-3.8549566
H	2.2867829	2.3491936	-5.7734986
H	0.3997020	4.0069114	-5.7228199
H	-1.1450905	4.0795798	-3.7432425
H	-0.7977290	2.5028749	-1.8197662
C	1.1209643	0.5937250	-1.6368683
C	1.2891557	-0.5235868	-1.0649263
H	1.3650205	-1.6113508	-1.0932481
H	-1.2044599	-1.9612831	1.7807001
C	-5.6935604	0.4280399	0.7868146
C	-4.8732260	1.5569739	0.6043783
C	-3.4791073	1.4241220	0.6323170
C	-3.7145290	-0.9672559	1.0353129
C	-5.1103379	-0.8335910	0.9991676
H	-6.7910934	0.5322035	0.7635136
H	-5.3271954	2.5483246	0.4407592
H	-2.8247368	2.2988518	0.4958738
H	-3.2728656	-1.9635792	1.1913143
H	-5.7485923	-1.7217179	1.1370152
C	3.0580331	-4.3695410	2.6573743
C	3.4298663	-3.0650970	3.0284627
C	2.6845134	-1.9624397	2.5882318
C	1.1570995	-3.4620276	1.4377184
C	1.9212272	-4.5624642	1.8534064
H	3.6573577	-5.2335446	2.9890534
H	4.3184064	-2.9022364	3.6605160
H	2.9930370	-0.9489848	2.8854907
H	0.2687670	-3.6236172	0.8047863
H	1.6251862	-5.5798783	1.5477199

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.34	0.18328	YES	YES
8	a	29.78	0.20821	YES	YES
9	a	32.91	0.04331	YES	YES
10	a	34.27	0.08747	YES	YES
11	a	41.54	0.19343	YES	YES
12	a	48.66	0.55510	YES	YES
13	a	57.82	0.19647	YES	YES
14	a	63.27	0.31881	YES	YES
15	a	74.34	0.11516	YES	YES
16	a	92.61	0.34213	YES	YES
17	a	95.48	0.14209	YES	YES
18	a	98.31	1.04767	YES	YES
19	a	104.50	0.24461	YES	YES
20	a	116.99	0.52529	YES	YES
21	a	124.52	0.20012	YES	YES
22	a	145.07	0.11716	YES	YES
23	a	154.08	0.65564	YES	YES
24	a	175.28	4.49094	YES	YES
25	a	193.75	0.92811	YES	YES
26	a	215.30	0.74143	YES	YES
27	a	221.97	0.42138	YES	YES
28	a	232.00	1.96209	YES	YES
29	a	259.41	0.65432	YES	YES
30	a	265.94	0.65064	YES	YES
31	a	318.81	19.77363	YES	YES
32	a	364.90	3.81450	YES	YES
33	a	396.90	1.90010	YES	YES
34	a	399.97	0.14845	YES	YES
35	a	401.99	0.35826	YES	YES
36	a	405.08	2.76880	YES	YES
37	a	417.70	8.06474	YES	YES
38	a	441.71	6.07106	YES	YES
39	a	453.03	1.48347	YES	YES
40	a	468.08	5.77371	YES	YES
41	a	476.58	1.52319	YES	YES
42	a	485.08	6.65317	YES	YES
43	a	488.75	9.69227	YES	YES
44	a	503.43	1.20446	YES	YES
45	a	509.22	27.45127	YES	YES
46	a	521.79	15.92382	YES	YES
47	a	534.58	10.70216	YES	YES
48	a	539.24	4.13881	YES	YES
49	a	563.79	5.43094	YES	YES
50	a	575.98	25.67458	YES	YES

3aa

SCF Energy (au) BP86/SV(P) -2427.897218753
SCF Energy (au) PBE0/def2-TZVPP -2427.461062227
SCF Energy (au) PBE0/def2-TZVPP -2427.4722378136 (Toluene Correction)
Zero Point Energy (au) 0.2981519
Chemical Potential (kJ mol^{-1}) 630.17
Dispersion Correction (au) PBE0/def2-TZVPP -0.06351537

xyz coordinates
43

Mn	1.1810811	0.7159650	0.5661474
C	1.6598767	0.9219215	2.3218986
C	2.8124931	0.1034934	0.0887737
C	1.6285850	2.3714621	0.1740137
O	1.8910188	3.4873282	-0.0653848
O	3.8664842	-0.2685205	-0.2369390
O	1.9970452	1.0639864	3.4301209
C	-1.3639759	0.0004371	1.3595888
C	-1.5344690	2.2323180	0.6746315
C	-2.8999818	2.2629891	0.9887676
C	-3.5043130	1.1126164	1.5220845
C	-2.7223835	-0.0387250	1.7130407
C	-0.4323711	-1.1556316	1.4903727
C	0.2282191	-1.6852839	0.3595376
C	0.9522997	-2.9703101	0.5092773
O	1.0602009	-3.4894198	1.8241345
C	0.4521165	-2.9346565	2.9014701
C	-0.3120505	-1.8039179	2.7701581
H	-1.0105112	3.1111142	0.2663304
H	-3.4764221	3.1855249	0.8182644
H	-4.5749929	1.1091453	1.7824192
H	-3.1549511	-0.9672730	2.1167805
O	1.4408513	-3.6214689	-0.3846887
C	0.7252502	-3.6793587	4.1700191
H	-0.7993238	-1.3709488	3.6556688
N	-0.7869478	1.1259126	0.8682712
C	0.4306811	0.7439951	-2.5882684
C	1.4333479	1.6346543	-3.0505655
C	1.3607196	2.2088200	-4.3280906
C	0.2732415	1.9259245	-5.1739001
C	-0.7390712	1.0556150	-4.7303850
C	-0.6602454	0.4704662	-3.4584866
H	2.2928458	1.8603887	-2.4004361
H	2.1611960	2.8881582	-4.6656384
H	0.2122367	2.3866509	-6.1738962
H	-1.6002679	0.8323011	-5.3826107
H	-1.4631317	-0.2007728	-3.1113904
C	0.5017330	0.1159829	-1.2647706
C	0.1302878	-1.1756697	-1.0245816
H	-0.0776536	-1.9218985	-1.8186780
H	0.1921505	-3.2179402	5.0253523
H	1.8172426	-3.6823528	4.3875594
H	0.4118588	-4.7430222	4.0740278

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-

6		0.00	0.00000	-	-
7	a	27.13	0.22894	YES	YES
8	a	31.31	1.15888	YES	YES
9	a	38.64	0.09170	YES	YES
10	a	47.06	3.23123	YES	YES
11	a	51.03	0.03444	YES	YES
12	a	65.80	0.31219	YES	YES
13	a	70.64	0.62300	YES	YES
14	a	83.70	0.71523	YES	YES
15	a	85.74	0.30667	YES	YES
16	a	98.66	0.91459	YES	YES
17	a	100.41	0.85868	YES	YES
18	a	105.58	0.32114	YES	YES
19	a	122.03	0.32392	YES	YES
20	a	142.13	0.21008	YES	YES
21	a	147.67	1.31379	YES	YES
22	a	154.77	0.60684	YES	YES
23	a	164.90	0.61796	YES	YES
24	a	168.59	1.02392	YES	YES
25	a	204.03	1.34226	YES	YES
26	a	234.09	0.82969	YES	YES
27	a	264.90	0.57805	YES	YES
28	a	271.62	0.42055	YES	YES
29	a	287.09	2.49634	YES	YES
30	a	306.14	0.94595	YES	YES
31	a	337.11	1.05520	YES	YES
32	a	370.70	2.97965	YES	YES
33	a	395.16	8.92298	YES	YES
34	a	408.27	0.68182	YES	YES
35	a	432.09	0.64404	YES	YES
36	a	450.92	2.19969	YES	YES
37	a	458.61	0.68661	YES	YES
38	a	471.99	2.82716	YES	YES
39	a	480.60	1.00547	YES	YES
40	a	486.92	0.72672	YES	YES
41	a	495.74	7.17728	YES	YES
42	a	498.30	3.06704	YES	YES
43	a	520.60	3.47485	YES	YES
44	a	534.57	2.34487	YES	YES
45	a	543.14	2.48022	YES	YES
46	a	552.57	3.12640	YES	YES
47	a	564.04	1.11003	YES	YES
48	a	599.29	2.19529	YES	YES
49	a	613.24	1.04141	YES	YES
50	a	616.73	25.69378	YES	YES

3aa'

SCF Energy (au) BP86/SV(P) -2427.892694005
SCF Energy (au) PBE0/def2-TZVPP -2427.457091685
SCF Energy (au) PBE0/def2-TZVPP -2427.4689841208 (Toluene Correction)
Zero Point Energy (au) 0.2981446
Chemical Potential (kJ mol^{-1}) 631.41
Dispersion Correction (au) PBE0/def2-TZVPP -0.06308410

xyz coordinates
43

Mn	1.3171493	1.8585225	0.5296280
C	1.6298756	2.1496790	2.3126624
C	3.0307253	1.3974938	0.2029409
C	1.6464497	3.5272692	0.0470398
O	1.8291102	4.6279022	-0.3021686
O	4.1385152	1.1270452	-0.0289385
O	1.8701931	2.3678615	3.4338012
C	-1.1847137	0.8917145	1.0692971
C	-1.5637281	3.1280814	0.5011556
C	-2.9455932	2.9756846	0.6882717
C	-3.4474210	1.7276430	1.0919780
C	-2.5502800	0.6634518	1.2902467
C	-0.0901566	-0.1110759	1.2427466
C	0.7083217	-0.4934816	0.1437899
C	1.7304981	-1.5486002	0.3443189
O	1.8298837	-2.0854507	1.6614893
C	1.0341846	-1.7118421	2.6908435
C	0.0741113	-0.7478401	2.5256006
H	-1.1168883	4.0879769	0.1958499
H	-3.6155793	3.8331442	0.5201520
H	-4.5283614	1.5817486	1.2486727
H	-2.8986445	-0.3336100	1.6009322
O	2.4712274	-2.0071104	-0.4899417
C	1.3433680	-2.4441814	3.9587961
H	-0.5466861	-0.4406024	3.3791964
N	-0.7096453	2.1048080	0.6960981
H	0.8184261	1.8829236	-2.3052401
C	0.8588862	1.3098571	-1.3604264
C	0.5171987	-0.0004278	-1.2695444
C	0.0323389	-0.9242508	-2.3214178
H	0.6553275	-2.1414774	4.7733723
H	2.3902219	-2.2377382	4.2764703
H	1.2642493	-3.5430963	3.8012614
C	-0.9610834	-2.6689967	-4.3362568
C	-0.2837614	-1.4860245	-4.6880366
C	0.2098940	-0.6288371	-3.6958179
C	-0.6469555	-2.1199279	-1.9851720
C	-1.1373039	-2.9824307	-2.9782057
H	-1.3423396	-3.3459983	-5.1185200
H	-0.1273649	-1.2356769	-5.7508757
H	0.7615512	0.2801757	-3.9854026
H	-0.8033312	-2.3761770	-0.9232676
H	-1.6618697	-3.9081283	-2.6873795

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-

6		0.00	0.00000	-	-
7	a	29.19	0.39689	YES	YES
8	a	37.85	0.18530	YES	YES
9	a	42.04	0.53987	YES	YES
10	a	45.28	2.33284	YES	YES
11	a	55.60	0.07883	YES	YES
12	a	71.08	1.12178	YES	YES
13	a	72.97	0.64680	YES	YES
14	a	81.99	0.64645	YES	YES
15	a	89.08	0.10909	YES	YES
16	a	92.22	0.21892	YES	YES
17	a	97.74	1.15302	YES	YES
18	a	104.90	0.38369	YES	YES
19	a	125.99	0.51286	YES	YES
20	a	140.22	2.69414	YES	YES
21	a	149.69	0.95855	YES	YES
22	a	161.56	1.03869	YES	YES
23	a	166.50	1.04911	YES	YES
24	a	189.68	0.39795	YES	YES
25	a	206.72	0.93187	YES	YES
26	a	226.68	0.48747	YES	YES
27	a	253.12	0.35894	YES	YES
28	a	281.86	1.61657	YES	YES
29	a	285.37	0.53583	YES	YES
30	a	303.63	3.70548	YES	YES
31	a	340.15	0.60494	YES	YES
32	a	346.30	1.04459	YES	YES
33	a	403.46	0.16006	YES	YES
34	a	423.67	1.61991	YES	YES
35	a	429.09	3.27110	YES	YES
36	a	452.70	3.31077	YES	YES
37	a	466.50	1.35906	YES	YES
38	a	473.72	1.84264	YES	YES
39	a	484.93	2.26677	YES	YES
40	a	487.33	1.39886	YES	YES
41	a	502.24	2.90579	YES	YES
42	a	519.55	11.89092	YES	YES
43	a	524.12	11.54128	YES	YES
44	a	535.06	2.93645	YES	YES
45	a	543.20	2.59277	YES	YES
46	a	556.86	3.38187	YES	YES
47	a	573.17	2.88697	YES	YES
48	a	600.66	33.06235	YES	YES
49	a	612.22	2.75040	YES	YES
50	a	619.54	32.55359	YES	YES

3ba

SCF Energy (au) BP86/SV(P) -2277.545461326
SCF Energy (au) PBE0/def2-TZVPP -2277.104429156
SCF Energy (au) PBE0/def2-TZVPP -2277.1124730146 (Toluene Correction)
Zero Point Energy (au) 0.2916084
Chemical Potential (kJ mol^{-1}) 622.44
Dispersion Correction (au) PBE0/def2-TZVPP -0.06485876

xyz coordinates
41

Mn	1.2035844	0.6105743	0.8523064
C	1.6744913	0.8965522	2.5994236
C	2.8473894	0.0456107	0.3779394
C	1.5909450	2.2597372	0.4049332
O	1.8148923	3.3744824	0.1207876
O	3.9082864	-0.3109878	0.0515739
O	2.0053768	1.0941946	3.7003449
C	-1.3227434	-0.2381294	1.6401022
C	-1.5436521	2.0144170	1.0274230
C	-2.9081022	2.0114590	1.3451955
C	-3.4882403	0.8327062	1.8409466
C	-2.6826732	-0.3079262	1.9888013
C	-0.3856671	-1.3933261	1.7627290
C	0.2684065	-1.9506208	0.6110439
C	1.0047266	-3.1538226	0.7947706
C	1.1268247	-3.7633542	2.0454734
C	0.5024462	-3.1928078	3.1746501
C	-0.2550789	-2.0287122	3.0254885
H	-1.0387463	2.9154439	0.6443993
H	-3.5013098	2.9283945	1.2048881
H	-4.5582313	0.7983263	2.1023647
H	-3.0974068	-1.2591955	2.3566214
H	1.4894977	-3.6036451	-0.0875664
H	1.7150206	-4.6901783	2.1489020
H	0.6024968	-3.6636841	4.1659042
H	-0.7641460	-1.5865805	3.8980022
N	-0.7722237	0.9178227	1.1841217
C	0.4618578	0.5683655	-2.2841753
C	1.4959925	1.4046476	-2.7766900
C	1.4177823	1.9803452	-4.0533923
C	0.2933206	1.7557737	-4.8679978
C	-0.7509429	0.9425426	-4.3928556
C	-0.6667157	0.3551167	-3.1214676
H	2.3837147	1.5872005	-2.1510279
H	2.2430676	2.6166848	-4.4145145
H	0.2281842	2.2194463	-5.8664202
H	-1.6426649	0.7667664	-5.0182869
H	-1.4952286	-0.2693487	-2.7481429
C	0.5384954	-0.0687245	-0.9602239
C	0.1581614	-1.3606470	-0.7491599
H	-0.1011875	-2.0549193	-1.5772156

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	30.29	0.17673	YES	YES

8	a	36.56	0.28054	YES	YES
9	a	45.25	0.15305	YES	YES
10	a	53.89	0.01637	YES	YES
11	a	59.66	0.18616	YES	YES
12	a	71.73	0.36929	YES	YES
13	a	75.91	0.28811	YES	YES
14	a	85.61	0.08148	YES	YES
15	a	95.08	1.34750	YES	YES
16	a	100.20	0.89084	YES	YES
17	a	106.07	0.11045	YES	YES
18	a	109.81	0.57321	YES	YES
19	a	145.93	0.39554	YES	YES
20	a	164.63	1.78407	YES	YES
21	a	176.37	0.65124	YES	YES
22	a	201.46	0.39912	YES	YES
23	a	225.54	0.91587	YES	YES
24	a	241.40	1.04718	YES	YES
25	a	290.50	0.84951	YES	YES
26	a	305.46	0.62450	YES	YES
27	a	340.85	1.99622	YES	YES
28	a	359.19	1.66423	YES	YES
29	a	407.29	0.27628	YES	YES
30	a	411.67	2.09351	YES	YES
31	a	430.32	2.45243	YES	YES
32	a	448.20	0.79627	YES	YES
33	a	458.90	0.39531	YES	YES
34	a	476.54	0.32414	YES	YES
35	a	479.07	5.08508	YES	YES
36	a	491.65	1.11876	YES	YES
37	a	505.52	7.79304	YES	YES
38	a	505.80	6.78980	YES	YES
39	a	534.99	0.55830	YES	YES
40	a	540.90	5.74478	YES	YES
41	a	548.34	4.66755	YES	YES
42	a	555.32	0.92651	YES	YES
43	a	564.16	0.93785	YES	YES
44	a	613.20	0.87636	YES	YES
45	a	621.73	35.32377	YES	YES
46	a	622.92	1.41328	YES	YES
47	a	630.49	26.57959	YES	YES
48	a	633.57	21.99769	YES	YES
49	a	644.97	6.16252	YES	YES
50	a	696.03	24.05804	YES	YES

3ba'

SCF Energy (au) BP86/SV(P) -2277.542842618
SCF Energy (au) PBE0/def2-TZVPP -2277.102650356
SCF Energy (au) PBE0/def2-TZVPP -2277.1108568307 (Toluene Correction)
Zero Point Energy (au) 0.2916320
Chemical Potential (kJ mol^{-1}) 621.89
Dispersion Correction (au) PBE0/def2-TZVPP -0.06426298

xyz coordinates
41

Mn	1.4885199	1.7045119	0.8181604
C	1.8265077	2.1026966	2.5777115
C	3.1454414	1.0652797	0.5205397
C	1.9444044	3.2939881	0.2327303
O	2.2063876	4.3558369	-0.1870421
O	4.2131739	0.6509773	0.3046883
O	2.0828108	2.3739325	3.6828999
C	-1.0888999	0.8846646	1.3480670
C	-1.2672276	3.1519178	0.7822458
C	-2.6578844	3.1277864	0.9576351
C	-3.2731840	1.9291202	1.3523987
C	-2.4749497	0.7898686	1.5512143
C	-0.1314261	-0.2465627	1.5563800
C	0.5976287	-0.8229594	0.4644390
C	1.4042200	-1.9613386	0.7375116
C	1.5023706	-2.5030140	2.0212514
C	0.7823654	-1.9282723	3.0902786
C	-0.0299553	-0.8176980	2.8543520
H	-0.7337819	4.0677567	0.4807180
H	-3.2445334	4.0438220	0.7866494
H	-4.3641253	1.8787612	1.4995791
H	-2.9143293	-0.1741581	1.8509878
H	1.9574847	-2.4179608	-0.0991123
H	2.1457900	-3.3806853	2.1980356
H	0.8584594	-2.3507146	4.1052713
H	-0.6028304	-0.3658125	3.6809242
N	-0.5072126	2.0562722	0.9820539
H	1.0338613	1.5503658	-1.9838215
C	0.9936968	1.0196038	-1.0131345
C	0.5364100	-0.2610022	-0.9328100
C	0.0626639	-1.1237395	-2.0460919
C	-0.8974941	-2.7471965	-4.1820293
C	-1.2411541	-3.0468770	-2.8531537
C	-0.7671295	-2.2467719	-1.8009977
C	0.4052510	-0.8428378	-3.3933402
C	-0.0706512	-1.6385431	-4.4441504
H	-1.2654379	-3.3762956	-5.0093935
H	-1.8885083	-3.9120274	-2.6308809
H	-1.0556802	-2.4909255	-0.7649647
H	1.0720201	0.0063175	-3.6141987
H	0.2169276	-1.3980867	-5.4816012

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	27.98	0.21003	YES	YES

8	a	35.88	0.03719	YES	YES
9	a	42.40	0.53053	YES	YES
10	a	53.71	0.17874	YES	YES
11	a	55.09	0.13841	YES	YES
12	a	75.80	0.23442	YES	YES
13	a	77.98	0.89256	YES	YES
14	a	86.90	0.33696	YES	YES
15	a	91.37	0.61055	YES	YES
16	a	95.14	0.10495	YES	YES
17	a	100.47	0.86115	YES	YES
18	a	108.09	0.34828	YES	YES
19	a	143.97	1.32281	YES	YES
20	a	172.24	0.81078	YES	YES
21	a	181.93	0.53638	YES	YES
22	a	212.56	0.77347	YES	YES
23	a	220.47	0.60037	YES	YES
24	a	260.51	0.31917	YES	YES
25	a	268.38	0.73732	YES	YES
26	a	316.09	0.36434	YES	YES
27	a	330.62	2.16754	YES	YES
28	a	355.25	0.15889	YES	YES
29	a	404.05	0.10322	YES	YES
30	a	415.22	2.55529	YES	YES
31	a	433.11	3.82045	YES	YES
32	a	454.83	1.38103	YES	YES
33	a	460.18	0.75567	YES	YES
34	a	471.42	3.55094	YES	YES
35	a	475.30	0.66048	YES	YES
36	a	491.02	1.76918	YES	YES
37	a	515.76	7.99125	YES	YES
38	a	517.19	10.00528	YES	YES
39	a	530.15	2.93397	YES	YES
40	a	543.68	6.69378	YES	YES
41	a	551.17	0.59449	YES	YES
42	a	572.72	7.04324	YES	YES
43	a	608.23	17.58280	YES	YES
44	a	612.63	17.55498	YES	YES
45	a	618.95	10.36268	YES	YES
46	a	624.31	3.62383	YES	YES
47	a	627.60	41.99112	YES	YES
48	a	636.32	10.37859	YES	YES
49	a	654.78	7.29210	YES	YES
50	a	693.78	26.60027	YES	YES

3bb

SCF Energy (au) BP86/SV(P) -2505.270959872
SCF Energy (au) PBE0/def2-TZVPP -2504.828741005
SCF Energy (au) PBE0/def2-TZVPP -2504.8384434576 (Toluene Correction)
Zero Point Energy (au) 0.3336560
Chemical Potential (kJ mol^{-1}) 711.91
Dispersion Correction (au) PBE0/def2-TZVPP -0.06961440

xyz coordinates
47
Mn 1.6477972 1.0275833 2.0605900
C 1.8976650 1.2694763 3.8608441
C 3.3020158 0.3626725 1.8050471
C 2.1780726 2.6512926 1.6683046
O 2.4926516 3.7462634 1.3914971
O 4.3695223 -0.0656815 1.6159589
O 2.0955334 1.4417486 4.9969535
C -0.9715380 0.2473441 2.4287731
C -1.0499351 2.5466755 1.9737597
C -2.4450362 2.5677129 2.1013274
C -3.1157768 1.3761657 2.4180761
C -2.3670369 0.1994742 2.5838918
C -0.0896805 -0.9507204 2.5898833
C 0.6469780 -1.4952711 1.4829103
C 1.2885120 -2.7487765 1.6746996
C 1.2464645 -3.4207830 2.8987807
C 0.5497269 -2.8619597 3.9908379
C -0.1201860 -1.6472937 3.8279927
H -0.4745746 3.4555027 1.7362322
H -2.9910714 3.5119022 1.9514598
H -4.2122378 1.3596749 2.5266123
H -2.8516628 -0.7613711 2.8163959
H 1.8354101 -3.1864927 0.8232017
H 1.7644995 -4.3876886 3.0112949
H 0.5233452 -3.3822485 4.9618903
H -0.6904628 -1.2151454 4.6669278
N -0.3372492 1.4146770 2.1450053
C 1.4343270 1.2627304 -1.0908466
C 1.2152329 0.4607538 0.1506046
C 0.7394831 -0.8075673 0.1684062
H 0.5149719 -1.3942259 -0.7454592
H 2.5194542 1.4570064 -1.2394867
O 1.0014743 0.5985720 -2.3075364
H 0.9106454 2.2410176 -1.0240664
C -0.2351374 0.9166963 -2.7772483
O -0.9697675 1.7454896 -2.2628037
C -0.5837036 0.1342317 -4.0072151
C -1.3420827 -1.2767439 -6.3226452
C -2.2212665 -0.3382637 -5.7518477
C -1.8439204 0.3645661 -4.5991023
C 0.2965975 -0.8071567 -4.5836955
C -0.0844649 -1.5091943 -5.7374509
H -1.6386221 -1.8296577 -7.2298127
H -3.2068873 -0.1543811 -6.2108652
H -2.5123797 1.1056769 -4.1330868
H 1.2790814 -0.9804965 -4.1195620
H 0.6052185 -2.2437876 -6.1854283

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-

3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.78	1.10029	YES	YES
8	a	21.30	0.05131	YES	YES
9	a	25.19	0.81352	YES	YES
10	a	39.40	0.01817	YES	YES
11	a	42.14	0.18979	YES	YES
12	a	55.45	0.68925	YES	YES
13	a	57.90	0.38211	YES	YES
14	a	64.94	0.45207	YES	YES
15	a	74.83	0.18833	YES	YES
16	a	83.62	0.12810	YES	YES
17	a	86.40	0.08338	YES	YES
18	a	93.65	1.00408	YES	YES
19	a	95.93	0.76442	YES	YES
20	a	107.74	0.05519	YES	YES
21	a	117.15	0.46782	YES	YES
22	a	146.24	0.38746	YES	YES
23	a	155.71	0.99850	YES	YES
24	a	175.99	1.34711	YES	YES
25	a	190.00	1.81081	YES	YES
26	a	214.51	0.56787	YES	YES
27	a	237.60	1.83998	YES	YES
28	a	276.57	2.56669	YES	YES
29	a	290.70	0.88472	YES	YES
30	a	311.95	3.93747	YES	YES
31	a	331.38	17.34403	YES	YES
32	a	354.47	0.52693	YES	YES
33	a	365.80	4.48850	YES	YES
34	a	374.44	1.17807	YES	YES
35	a	404.85	0.01467	YES	YES
36	a	434.65	1.57511	YES	YES
37	a	441.25	0.43459	YES	YES
38	a	446.29	0.05822	YES	YES
39	a	455.43	0.59858	YES	YES
40	a	466.19	2.35891	YES	YES
41	a	475.71	2.30286	YES	YES
42	a	477.44	2.93109	YES	YES
43	a	489.91	1.94362	YES	YES
44	a	495.82	6.22667	YES	YES
45	a	511.62	5.83307	YES	YES
46	a	522.82	10.20532	YES	YES
47	a	538.10	1.68865	YES	YES
48	a	549.48	1.99689	YES	YES
49	a	576.38	3.85253	YES	YES
50	a	610.28	0.55554	YES	YES

3bb'

SCF Energy (au) BP86/SV(P) -2505.262474030
SCF Energy (au) PBE0/def2-TZVPP -2504.821881763
SCF Energy (au) PBE0/def2-TZVPP -2504.8324982709 (Toluene Correction)
Zero Point Energy (au) 0.3332973
Chemical Potential (kJ mol^{-1}) 707.95
Dispersion Correction (au) PBE0/def2-TZVPP -0.06822560

xyz coordinates
47

Mn	1.4239376	1.6744286	1.8220771
C	1.8865455	2.2627008	3.4965058
C	3.1056942	1.2035792	1.3873430
C	1.6306999	3.2445483	1.0746210
O	1.7262686	4.2893934	0.5526978
O	4.1875927	0.8961212	1.0815572
O	2.2210702	2.6565818	4.5424955
C	-0.9950372	0.6248463	2.6735470
C	-1.4576079	2.8078057	1.9592185
C	-2.8176036	2.6651682	2.2663124
C	-3.2690759	1.4505949	2.8065614
C	-2.3417691	0.4156411	3.0134971
C	0.0764247	-0.3995511	2.8792772
C	0.7681943	-0.9957410	1.7734712
C	1.6808274	-2.0469290	2.0566569
C	1.9203980	-2.4827095	3.3635035
C	1.2444886	-1.8825392	4.4449250
C	0.3280167	-0.8567160	4.1995850
H	-1.0510607	3.7420424	1.5401705
H	-3.5079445	3.5031200	2.0827257
H	-4.3320018	1.3072214	3.0598091
H	-2.6511245	-0.5576994	3.4248795
H	2.2192233	-2.5183200	1.2184258
H	2.6446682	-3.2935919	3.5462002
H	1.4342444	-2.2179514	5.4773143
H	-0.2138813	-0.3881755	5.0377423
N	-0.5713820	1.8119713	2.1663599
H	0.7444662	1.1648687	-0.9101610
C	0.8359730	0.7575780	0.1133129
C	0.5410352	-0.5397815	0.3604814
C	0.0598516	-1.5885711	-0.6198576
H	0.7383530	-2.4730668	-0.6561824
O	-0.0366306	-1.0211831	-1.9346468
H	-0.9394416	-1.9890683	-0.3240467
C	-0.3792417	-1.8897228	-2.9238423
C	-0.4612079	-1.2276167	-4.2638339
O	-0.5948285	-3.0752282	-2.7243464
C	-0.6481598	-0.0957918	-6.8346892
C	-0.2881988	0.7066557	-5.7371038
C	-0.1944030	0.1455912	-4.4542450
C	-0.8217122	-2.0287012	-5.3688646
C	-0.9151381	-1.4646325	-6.6486519
H	-0.7204377	0.3484577	-7.8416054
H	-0.0772928	1.7790471	-5.8830349
H	0.0882734	0.7675542	-3.5916822
H	-1.0240530	-3.0975207	-5.1960703
H	-1.1970123	-2.0947084	-7.5084098

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	4.99	0.87779	YES	YES
8	a	14.98	0.49000	YES	YES
9	a	27.14	0.57272	YES	YES
10	a	41.47	0.03971	YES	YES
11	a	43.34	0.10929	YES	YES
12	a	50.05	0.78132	YES	YES
13	a	62.65	1.08905	YES	YES
14	a	73.73	0.24892	YES	YES
15	a	76.33	0.74414	YES	YES
16	a	80.36	0.19552	YES	YES
17	a	93.09	0.68049	YES	YES
18	a	93.15	0.12074	YES	YES
19	a	97.84	0.99353	YES	YES
20	a	107.09	0.42463	YES	YES
21	a	113.49	0.31746	YES	YES
22	a	138.60	0.77426	YES	YES
23	a	163.63	2.56034	YES	YES
24	a	165.67	1.61550	YES	YES
25	a	186.51	1.09764	YES	YES
26	a	199.15	1.39561	YES	YES
27	a	209.75	1.17396	YES	YES
28	a	255.17	3.35363	YES	YES
29	a	265.72	1.06408	YES	YES
30	a	299.42	3.21550	YES	YES
31	a	320.48	2.42530	YES	YES
32	a	331.95	3.75774	YES	YES
33	a	364.98	1.97094	YES	YES
34	a	379.24	1.10255	YES	YES
35	a	403.35	0.00028	YES	YES
36	a	434.60	4.97223	YES	YES
37	a	445.03	0.12190	YES	YES
38	a	451.78	0.68727	YES	YES
39	a	458.23	2.59165	YES	YES
40	a	474.34	0.99981	YES	YES
41	a	479.67	3.72907	YES	YES
42	a	482.22	7.97386	YES	YES
43	a	491.27	4.35792	YES	YES
44	a	515.35	9.18263	YES	YES
45	a	525.91	1.57433	YES	YES
46	a	529.50	3.93818	YES	YES
47	a	538.23	2.59232	YES	YES
48	a	562.36	3.58769	YES	YES
49	a	564.16	4.23410	YES	YES
50	a	610.15	0.24927	YES	YES

3bc

SCF Energy (au) BP86/SV(P)	-2281.135995277
SCF Energy (au) PBE0/def2-TZVPP	-2280.709892308
SCF Energy (au) PBE0/def2-TZVPP	-2280.7163380043 (Toluene Correction)
Zero Point Energy (au)	0.3591834
Chemical Potential (kJ mol^{-1})	796.63
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07061984

xyz coordinates
47

Mn	0.9786078	0.4084770	1.2223343
C	1.4551385	0.7317916	2.9633209
C	2.6487590	-0.0631594	0.7487877
C	1.2731209	2.0653396	0.7424884
O	1.4452458	3.1841802	0.4315049
O	3.7297294	-0.3705447	0.4367893
O	1.7956414	0.9609250	4.0552737
C	-1.4787280	-0.6152415	2.0577329
C	-1.8374708	1.6433332	1.5472334
C	-3.1878842	1.5579354	1.9092559
C	-3.6919294	0.3292394	2.3653486
C	-2.8228319	-0.7705066	2.4414410
C	-0.4767104	-1.7177011	2.1490224
C	0.2007391	-2.2195548	0.9882094
C	1.0166975	-3.3725104	1.1547545
C	1.1880167	-3.9861117	2.3980705
C	0.5382259	-3.4679615	3.5375738
C	-0.2931455	-2.3530503	3.4052073
H	-1.3909560	2.5879543	1.1990451
H	-3.8287663	2.4500780	1.8344837
H	-4.7498712	0.2270415	2.6566231
H	-3.1740538	-1.7555089	2.7856520
H	1.5223039	-3.7814818	0.2641371
H	1.8355437	-4.8741353	2.4873512
H	0.6770980	-3.9400769	4.5235565
H	-0.8203979	-1.9511518	4.2863317
N	-1.0056886	0.5825233	1.6225377
C	0.3155452	0.2669481	-1.9794547
C	0.3573697	-0.3225684	-0.5901665
C	0.0442766	-1.6255992	-0.3677651
H	-0.2105193	-2.3278742	-1.1932185
C	1.7013136	0.7314648	-2.4901721
H	-0.0187280	-0.5468414	-2.6714409
C	-0.7056419	1.4391834	-2.1074004
H	2.0152261	1.6281379	-1.9101778
C	1.6581457	1.0609065	-4.0037239
H	2.4660993	-0.0490734	-2.2881233
C	-0.3841621	2.3961246	-3.2829140
H	-0.7203774	2.0173101	-1.1577774
H	-1.7261741	1.0089775	-2.2249673
C	0.2917179	1.6487285	-4.4435602
H	0.2940312	3.2084799	-2.9339137
H	-1.3148005	2.8999546	-3.6280212
H	2.4749332	1.7797358	-4.2395862
H	1.8751732	0.1435980	-4.5970909
H	0.4245959	2.3216262	-5.3197810
H	-0.3844579	0.8306588	-4.7848120

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	35.36	0.26877	YES	YES
8	a	37.03	0.11738	YES	YES
9	a	48.25	0.04837	YES	YES
10	a	51.60	0.02182	YES	YES
11	a	60.04	0.43157	YES	YES
12	a	65.10	0.52792	YES	YES
13	a	76.48	0.13860	YES	YES
14	a	88.60	0.05733	YES	YES
15	a	96.20	0.79255	YES	YES
16	a	100.71	0.79076	YES	YES
17	a	107.42	0.45034	YES	YES
18	a	108.57	0.28856	YES	YES
19	a	123.15	0.04763	YES	YES
20	a	142.86	0.45196	YES	YES
21	a	161.33	1.25089	YES	YES
22	a	171.62	0.05950	YES	YES
23	a	187.52	0.39619	YES	YES
24	a	212.63	1.39349	YES	YES
25	a	223.89	0.51838	YES	YES
26	a	259.86	0.08106	YES	YES
27	a	290.14	1.01879	YES	YES
28	a	295.14	1.52142	YES	YES
29	a	333.21	1.70194	YES	YES
30	a	355.39	1.34461	YES	YES
31	a	403.43	0.50782	YES	YES
32	a	419.53	7.20342	YES	YES
33	a	443.13	1.20729	YES	YES
34	a	451.04	0.97650	YES	YES
35	a	462.27	1.80215	YES	YES
36	a	464.56	0.30656	YES	YES
37	a	473.55	0.91469	YES	YES
38	a	481.66	5.21201	YES	YES
39	a	493.70	2.55763	YES	YES
40	a	503.71	8.88712	YES	YES
41	a	510.53	8.46111	YES	YES
42	a	528.20	0.73778	YES	YES
43	a	537.71	0.57584	YES	YES
44	a	548.05	1.17087	YES	YES
45	a	550.95	2.53395	YES	YES
46	a	567.38	2.39919	YES	YES
47	a	621.92	28.41054	YES	YES
48	a	622.65	2.27148	YES	YES
49	a	629.06	34.34545	YES	YES
50	a	634.10	7.22001	YES	YES

3bc'

SCF Energy (au) BP86/SV(P)	-2281.140662981
SCF Energy (au) PBE0/def2-TZVPP	-2280.715719323
SCF Energy (au) PBE0/def2-TZVPP	-2280.7223820342 (Toluene Correction)
Zero Point Energy (au)	0.3590261
Chemical Potential (kJ mol^{-1})	795.17
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06962776

xyz coordinates
47

Mn	1.7008294	1.9178340	1.2440537
C	1.9464929	2.2382414	3.0331653
C	3.3315730	1.1960531	1.0180863
C	2.2868389	3.4888898	0.7343215
O	2.6405981	4.5418127	0.3602348
O	4.3846566	0.7258024	0.8452115
O	2.1525111	2.4639907	4.1595807
C	-0.9782636	1.2554733	1.5666412
C	-0.9342414	3.5476428	1.0845970
C	-2.3307824	3.6335022	1.1661203
C	-3.0673510	2.4772899	1.4704893
C	-2.3784885	1.2697402	1.6733330
C	-0.1295595	0.0478783	1.8081275
C	0.6845288	-0.5178141	0.7703939
C	1.4519761	-1.6688415	1.1034235
C	1.3975069	-2.2547954	2.3717161
C	0.5680687	-1.7075987	3.3710144
C	-0.1827243	-0.5644054	3.0883288
H	-0.3100682	4.4267213	0.8574934
H	-2.8276646	4.6011997	0.9947426
H	-4.1662721	2.5132506	1.5450442
H	-2.9131136	0.3353467	1.9044298
H	2.1172542	-2.0946194	0.3373892
H	2.0127821	-3.1433835	2.5897974
H	0.5222532	-2.1657562	4.3723103
H	-0.8209259	-0.1154719	3.8673750
N	-0.2777518	2.3872866	1.2903563
H	1.3996283	1.8612120	-1.6028164
C	1.2783893	1.3182463	-0.6440395
C	0.7292965	0.0806393	-0.6157631
C	0.1674180	-0.6703298	-1.8229329
C	0.9487741	-1.9443464	-2.2328460
H	0.2553998	0.0463469	-2.6744401
C	-1.3354527	-1.0109098	-1.6610256
H	2.0263430	-1.6978684	-2.3658397
C	0.3755887	-2.5712595	-3.5174003
H	0.8866761	-2.6995264	-1.4142843
C	-1.9210119	-1.6584808	-2.9299712
H	-1.9023449	-0.0867089	-1.4056220
H	-1.4595226	-1.7099529	-0.7988130
C	-1.1197359	-2.8983627	-3.3627757
H	-1.9112953	-0.9089820	-3.7575255
H	-2.9896957	-1.9259817	-2.7643687
H	0.9474940	-3.4898021	-3.7824158
H	0.5125164	-1.8597757	-4.3661075
H	-1.5283127	-3.3092554	-4.3136337
H	-1.2408158	-3.7001716	-2.5951562

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.50	0.32533	YES	YES
8	a	31.99	0.01860	YES	YES
9	a	44.13	0.24008	YES	YES
10	a	51.06	0.22408	YES	YES
11	a	51.84	0.35126	YES	YES
12	a	69.06	0.38263	YES	YES
13	a	77.41	0.09042	YES	YES
14	a	87.88	0.23113	YES	YES
15	a	93.53	0.67250	YES	YES
16	a	96.45	0.52594	YES	YES
17	a	100.05	0.08474	YES	YES
18	a	106.99	0.49804	YES	YES
19	a	131.13	0.27875	YES	YES
20	a	157.94	0.90602	YES	YES
21	a	169.99	1.48451	YES	YES
22	a	203.07	0.56503	YES	YES
23	a	210.99	0.25113	YES	YES
24	a	220.28	0.40385	YES	YES
25	a	238.63	0.03352	YES	YES
26	a	268.33	0.02872	YES	YES
27	a	306.85	0.86862	YES	YES
28	a	314.02	0.39462	YES	YES
29	a	337.59	1.09218	YES	YES
30	a	353.62	1.49040	YES	YES
31	a	389.14	0.87982	YES	YES
32	a	428.20	1.24568	YES	YES
33	a	436.17	3.80539	YES	YES
34	a	439.55	1.18578	YES	YES
35	a	458.00	1.66801	YES	YES
36	a	463.29	0.79979	YES	YES
37	a	471.05	1.32839	YES	YES
38	a	476.24	1.22475	YES	YES
39	a	491.21	2.23124	YES	YES
40	a	515.51	7.94809	YES	YES
41	a	518.27	3.62172	YES	YES
42	a	522.65	6.67053	YES	YES
43	a	537.87	3.65551	YES	YES
44	a	546.13	2.31482	YES	YES
45	a	582.34	2.57348	YES	YES
46	a	604.22	21.23873	YES	YES
47	a	620.00	8.90392	YES	YES
48	a	627.22	38.83376	YES	YES
49	a	629.79	7.92577	YES	YES
50	a	637.71	8.14397	YES	YES

3bd

SCF Energy (au) BP86/SV(P)	-2411.413617596
SCF Energy (au) PBE0/def2-TZVPP	-2410.960779076
SCF Energy (au) PBE0/def2-TZVPP	-2410.9697888395 (Toluene Correction)
Zero Point Energy (au)	0.3619092
Chemical Potential (kJ mol^{-1})	789.69
Dispersion Correction (au)PBE0/def2-TZVPP	-0.07292669

xyz coordinates

49			
Mn	1.1580946	0.2533469	2.0022092
C	1.6348367	0.5380953	3.7484200
C	2.7925991	-0.3277689	1.5176508
C	1.5653154	1.8951322	1.5564534
O	1.8040972	3.0097385	1.2778736
O	3.8473452	-0.6948563	1.1821893
O	1.9709921	0.7309954	4.8490138
C	-1.4026967	-0.5179689	2.8343411
C	-1.5531558	1.7099038	2.1187935
C	-2.9141328	1.7686986	2.4427297
C	-3.5306391	0.6351080	2.9973705
C	-2.7627536	-0.5232472	3.1929938
C	-0.5156184	-1.7030816	2.9964020
C	0.1482835	-2.2987802	1.8677420
C	0.8337906	-3.5265776	2.0928654
C	0.9013429	-4.1209366	3.3544102
C	0.2704004	-3.5108000	4.4591501
C	-0.4399921	-2.3227292	4.2706203
H	-1.0218140	2.5749738	1.6915378
H	-3.4766530	2.6978981	2.2619131
H	-4.5994638	0.6490149	3.2655475
H	-3.2072983	-1.4427180	3.6042513
H	1.3250606	-4.0080314	1.2309236
H	1.4531173	-5.0665573	3.4859650
H	0.3288523	-3.9680692	5.4600933
H	-0.9536017	-1.8474087	5.1229669
N	-0.8152995	0.5974297	2.3241413
C	0.4378693	0.0965152	-1.1362323
C	1.4061952	1.0155642	-1.6139407
C	1.3827041	1.5187134	-2.9174912
C	0.3575769	1.1454161	-3.8349631
C	-0.6344641	0.2388594	-3.3574599
C	-0.5845963	-0.2648783	-2.0551730
H	2.2229875	1.3305442	-0.9460467
H	2.1765766	2.2157761	-3.2215062
N	0.3208918	1.6473731	-5.1284990
H	-1.4644746	-0.0724593	-4.0085269
H	-1.3814464	-0.9508668	-1.7224392
C	0.4823353	-0.4694157	0.2148392
C	0.0874268	-1.7501554	0.4903919
H	-0.1313716	-2.4849103	-0.3141261
C	-0.7211384	1.2196232	-6.0429968
C	1.3460939	2.5724649	-5.5760493
H	1.3697334	3.5021422	-4.9580529
H	1.1409724	2.8697347	-6.6241407
H	2.3674314	2.1205057	-5.5435120
H	-0.5728768	1.7113929	-7.0250688
H	-1.7409551	1.4924086	-5.6775268
H	-0.7084804	0.1148478	-6.2100478

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	21.08	0.31267	YES	YES
8	a	25.20	1.16210	YES	YES
9	a	39.43	0.37353	YES	YES
10	a	43.29	0.93927	YES	YES
11	a	49.24	0.06683	YES	YES
12	a	55.98	0.63821	YES	YES
13	a	65.09	0.47275	YES	YES
14	a	74.16	0.64624	YES	YES
15	a	75.81	0.02333	YES	YES
16	a	85.58	0.10151	YES	YES
17	a	93.05	2.03898	YES	YES
18	a	98.03	0.55357	YES	YES
19	a	100.07	1.20359	YES	YES
20	a	107.45	0.07850	YES	YES
21	a	121.05	0.15239	YES	YES
22	a	134.11	0.51650	YES	YES
23	a	153.22	1.04832	YES	YES
24	a	174.25	0.48049	YES	YES
25	a	197.72	1.30506	YES	YES
26	a	213.05	0.33096	YES	YES
27	a	214.24	1.50010	YES	YES
28	a	222.78	0.43599	YES	YES
29	a	261.15	3.97850	YES	YES
30	a	287.96	1.54180	YES	YES
31	a	300.00	6.92838	YES	YES
32	a	309.55	1.05348	YES	YES
33	a	351.99	0.36710	YES	YES
34	a	365.35	3.37415	YES	YES
35	a	411.90	2.31770	YES	YES
36	a	419.13	3.32007	YES	YES
37	a	423.46	0.65970	YES	YES
38	a	443.47	1.55412	YES	YES
39	a	455.43	1.10299	YES	YES
40	a	462.10	0.58427	YES	YES
41	a	469.99	3.00002	YES	YES
42	a	477.73	5.04355	YES	YES
43	a	483.03	11.93955	YES	YES
44	a	492.17	1.18165	YES	YES
45	a	505.41	6.49846	YES	YES
46	a	511.22	3.50146	YES	YES
47	a	532.30	1.08792	YES	YES
48	a	539.35	4.13962	YES	YES
49	a	541.66	10.15662	YES	YES
50	a	553.79	0.72502	YES	YES

3bd'

SCF Energy (au) BP86/SV(P)	-2411.410447430
SCF Energy (au) PBE0/def2-TZVPP	-2410.9683234203
SCF Energy (au) PBE0/def2-TZVPP	-2410.958998524 (Toluene Correction)
Zero Point Energy (au)	0.3619800
Chemical Potential (kJ mol^{-1})	789.09
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07249849

xyz coordinates

49			
Mn	1.7594811	2.3780870	1.7905522
C	2.1164445	2.7676239	3.5463937
C	3.4076023	1.7338603	1.4632533
C	2.2143365	3.9673582	1.2063758
O	2.4755736	5.0305307	0.7878539
O	4.4702473	1.3172361	1.2254476
O	2.3853366	3.0343150	4.6505127
C	-0.8169518	1.5653483	2.3349170
C	-0.9917541	3.8351141	1.7792212
C	-2.3812763	3.8152428	1.9639769
C	-2.9979374	2.6172537	2.3586792
C	-2.2019531	1.4746599	2.5473014
C	0.1367893	0.4292305	2.5314332
C	0.8530995	-0.1481106	1.4311450
C	1.6521145	-1.2944059	1.6949435
C	1.7573642	-1.8404689	2.9760550
C	1.0507163	-1.2637499	4.0532881
C	0.2446318	-0.1468652	3.8269131
H	-0.4570121	4.7502102	1.4776112
H	-2.9658978	4.7340201	1.8005746
H	-4.0880015	2.5700200	2.5135215
H	-2.6421761	0.5107777	2.8463223
H	2.1936939	-1.7523399	0.8514653
H	2.3962216	-2.7231491	3.1449226
H	1.1324764	-1.6894560	5.0665279
H	-0.3183687	0.3068091	4.6593589
N	-0.2338650	2.7364166	1.9696384
H	1.2873711	2.2305719	-1.0112830
C	1.2436783	1.6982825	-0.0416089
C	0.7855325	0.4171385	0.0359651
C	0.3205685	-0.4499935	-1.0740953
C	-0.6403717	-2.1028271	-3.2470443
C	-0.9730280	-2.3859338	-1.8917463
C	-0.5033633	-1.5792577	-0.8481322
C	0.6575204	-0.1811621	-2.4238388
C	0.1967957	-0.9714930	-3.4795579
N	-1.1012140	-2.8933772	-4.2925653
H	-1.6118688	-3.2452270	-1.6415554
H	-0.8003567	-1.8353762	0.1830288
H	1.3209240	0.6686278	-2.6539594
H	0.5086177	-0.7108120	-4.5012067
C	-0.7156781	-2.5868255	-5.6574505
C	-1.9011040	-4.0696289	-4.0099143
H	-1.3570415	-4.8108492	-3.3737167
H	-2.1675748	-4.5714991	-4.9617157
H	-2.8533116	-3.8128451	-3.4853204
H	-1.0397056	-1.5628749	-5.9622423
H	-1.1969285	-3.3097895	-6.3461398
H	0.3896025	-2.6504176	-5.8141060

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.99	0.66596	YES	YES
8	a	27.88	0.03399	YES	YES
9	a	33.40	0.36254	YES	YES
10	a	42.85	0.76193	YES	YES
11	a	51.37	0.25743	YES	YES
12	a	53.18	0.34361	YES	YES
13	a	67.75	1.47722	YES	YES
14	a	73.69	0.26541	YES	YES
15	a	78.21	0.05442	YES	YES
16	a	79.66	0.15106	YES	YES
17	a	85.98	0.22070	YES	YES
18	a	91.80	0.36237	YES	YES
19	a	96.10	1.06830	YES	YES
20	a	100.26	0.00276	YES	YES
21	a	125.52	1.17836	YES	YES
22	a	136.18	0.61147	YES	YES
23	a	165.06	0.63800	YES	YES
24	a	188.52	0.75308	YES	YES
25	a	194.01	1.12099	YES	YES
26	a	200.97	0.76149	YES	YES
27	a	215.44	0.05230	YES	YES
28	a	225.48	0.35162	YES	YES
29	a	262.85	0.32014	YES	YES
30	a	285.40	0.22519	YES	YES
31	a	304.78	1.10759	YES	YES
32	a	318.87	3.40583	YES	YES
33	a	351.60	0.75539	YES	YES
34	a	359.42	1.44456	YES	YES
35	a	386.42	0.45695	YES	YES
36	a	419.25	0.06425	YES	YES
37	a	430.54	2.55204	YES	YES
38	a	435.88	3.72607	YES	YES
39	a	457.39	1.39231	YES	YES
40	a	465.04	0.70328	YES	YES
41	a	474.90	1.30233	YES	YES
42	a	477.20	5.66843	YES	YES
43	a	489.75	4.52679	YES	YES
44	a	507.07	4.70699	YES	YES
45	a	515.39	6.35917	YES	YES
46	a	519.83	12.09470	YES	YES
47	a	528.54	3.87924	YES	YES
48	a	540.13	3.23204	YES	YES
49	a	545.49	2.69293	YES	YES
50	a	565.39	3.44381	YES	YES

3be

SCF Energy (au) BP86/SV(P) -2391.988619360
SCF Energy (au) PBE0/def2-TZVPP -2391.5574436897
SCF Energy (au) PBE0/def2-TZVPP -2391.548466315 (Toluene Correction)
Zero Point Energy (au) 0.3230463
Chemical Potential (kJ mol^{-1}) 696.07
Dispersion Correction (au) PBE0/def2-TZVPP -0.06844294

xyz coordinates
45

Mn	1.0783337	0.3015995	1.4730911
C	1.5331549	0.5569657	3.2296976
C	2.7235407	-0.2613077	1.0018111
C	1.4768076	1.9552219	1.0594871
O	1.7082128	3.0750269	0.7988311
O	3.7858959	-0.6148355	0.6762550
O	1.8555017	0.7340766	4.3367940
C	-1.4676057	-0.5315029	2.2360618
C	-1.6583114	1.7225253	1.6187454
C	-3.0252121	1.7354861	1.9244400
C	-3.6228405	0.5642922	2.4176952
C	-2.8313094	-0.5847469	2.5738154
C	-0.5484364	-1.6989853	2.3623694
C	0.1181285	-2.2516676	1.2147237
C	0.8344046	-3.4674634	1.3995329
C	0.9270770	-4.0918218	2.6452063
C	0.2919355	-3.5247154	3.7702885
C	-0.4474334	-2.3491377	3.6201287
H	-1.1404232	2.6174085	1.2388200
H	-3.6069078	2.6586850	1.7769019
H	-4.6953745	0.5422602	2.6698833
H	-3.2598795	-1.5310727	2.9384950
H	1.3282009	-3.9147031	0.5208648
H	1.5012311	-5.0275059	2.7482383
H	0.3695262	-4.0067391	4.7581991
H	-0.9650548	-1.9088440	4.4885654
N	-0.8997333	0.6179357	1.7841440
C	0.3727864	0.2770489	-1.6717431
C	1.3747366	1.1671111	-2.1257371
C	1.3339791	1.7492282	-3.4028118
C	0.2552050	1.4697441	-4.2693719
C	-0.7677767	0.5961581	-3.8328035
C	-0.7039282	0.0129448	-2.5661651
H	2.2277463	1.3973128	-1.4688332
H	2.1476028	2.4240561	-3.7073650
O	0.1054240	1.9924912	-5.5212622
H	-1.6110245	0.3972062	-4.5133675
H	-1.5184473	-0.6533929	-2.2376011
C	0.4281146	-0.3617485	-0.3500053
C	0.0371062	-1.6531094	-0.1424265
H	-0.2044882	-2.3468740	-0.9762725
C	1.0986463	2.8748195	-6.0115048
H	0.7745559	3.1690357	-7.0304530
H	2.0975340	2.3808154	-6.0755190
H	1.1887987	3.7907179	-5.3798433

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	24.73	0.42575	YES	YES
8	a	32.77	0.77416	YES	YES
9	a	42.59	0.15089	YES	YES
10	a	46.02	0.87848	YES	YES
11	a	52.13	0.24975	YES	YES
12	a	63.43	0.74685	YES	YES
13	a	74.81	0.35220	YES	YES
14	a	85.09	0.23384	YES	YES
15	a	92.76	2.26815	YES	YES
16	a	96.37	0.91130	YES	YES
17	a	99.38	0.70388	YES	YES
18	a	107.24	0.04566	YES	YES
19	a	110.33	0.13395	YES	YES
20	a	134.31	0.77873	YES	YES
21	a	149.52	0.77319	YES	YES
22	a	156.88	0.95919	YES	YES
23	a	184.06	2.13859	YES	YES
24	a	207.19	1.35787	YES	YES
25	a	225.26	0.81501	YES	YES
26	a	245.18	1.33807	YES	YES
27	a	261.34	0.08205	YES	YES
28	a	288.42	1.41136	YES	YES
29	a	299.88	4.71848	YES	YES
30	a	309.29	1.51426	YES	YES
31	a	355.99	0.36497	YES	YES
32	a	374.05	3.39132	YES	YES
33	a	416.53	2.14670	YES	YES
34	a	420.58	1.90198	YES	YES
35	a	442.85	1.75952	YES	YES
36	a	449.83	0.82556	YES	YES
37	a	458.49	1.00003	YES	YES
38	a	460.39	0.68765	YES	YES
39	a	477.03	2.82516	YES	YES
40	a	481.12	4.21536	YES	YES
41	a	491.75	0.15798	YES	YES
42	a	505.02	7.51385	YES	YES
43	a	510.10	5.19666	YES	YES
44	a	531.44	9.00323	YES	YES
45	a	539.68	6.37763	YES	YES
46	a	543.52	12.21052	YES	YES
47	a	553.19	0.47352	YES	YES
48	a	562.70	0.53993	YES	YES
49	a	606.89	11.00156	YES	YES
50	a	622.36	39.86735	YES	YES

3be'

SCF Energy (au) BP86/SV(P) -2391.985428432
SCF Energy (au) PBE0/def2-TZVPP -2391.546398574
SCF Energy (au) PBE0/def2-TZVPP -2391.5556957408 (Toluene Correction)
Zero Point Energy (au) 0.3230217
Chemical Potential (kJ mol^{-1}) 695.14
Dispersion Correction (au) PBE0/def2-TZVPP -0.06784260

xyz coordinates
45

Mn	1.8122988	1.9480148	1.4147212
C	2.1633410	2.2412118	3.1914086
C	3.4260367	1.2198082	1.0881766
C	2.3708124	3.5311227	0.9087900
O	2.7033871	4.5923569	0.5400796
O	4.4661979	0.7486149	0.8543723
O	2.4275983	2.4515952	4.3083436
C	-0.8078624	1.2543860	1.8906140
C	-0.8508899	3.5589190	1.4669078
C	-2.2403562	3.6070803	1.6471064
C	-2.9257347	2.4251631	1.9702234
C	-2.1967927	1.2302014	2.0941101
C	0.0787136	0.0554271	2.0244011
C	0.7642242	-0.5020519	0.8946779
C	1.4890464	-1.7088776	1.0928999
C	1.5535021	-2.3326115	2.3409788
C	0.8802061	-1.7743965	3.4486059
C	0.1461699	-0.5981896	3.2855988
H	-0.2635877	4.4578431	1.2194019
H	-2.7712795	4.5655252	1.5367376
H	-4.0175570	2.4309466	2.1193480
H	-2.6923763	0.2773633	2.3364265
H	2.0070467	-2.1502731	0.2261206
H	2.1351046	-3.2617665	2.4597967
H	0.9310593	-2.2610244	4.4360588
H	-0.3910429	-0.1582303	4.1420564
N	-0.1578763	2.4098254	1.5956229
H	1.3664242	1.9902530	-1.3918890
C	1.2834493	1.4028131	-0.4572734
C	0.7459051	0.1509559	-0.4625141
C	0.2320746	-0.6098678	-1.6295954
C	-0.8102307	-2.0339223	-3.8802903
C	-1.1850094	-2.3990410	-2.5709966
C	-0.6648818	-1.6912546	-1.4726317
C	0.5997018	-0.2684207	-2.9589371
C	0.0913856	-0.9579672	-4.0595924
O	-1.2465295	-2.6482198	-5.0190950
H	-1.8836455	-3.2294423	-2.3891168
H	-0.9813916	-1.9900963	-0.4593405
H	1.3172506	0.5508679	-3.1272071
H	0.3890617	-0.6920816	-5.0863897
C	-2.1423304	-3.7371722	-4.8997078
H	-3.0985747	-3.4365554	-4.4077426
H	-1.6928093	-4.5843190	-4.3276767
H	-2.3592397	-4.0745133	-5.9335893

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.52	0.30109	YES	YES
8	a	30.01	0.16593	YES	YES
9	a	36.90	0.27643	YES	YES
10	a	50.51	0.06423	YES	YES
11	a	52.27	0.21524	YES	YES
12	a	67.09	1.22178	YES	YES
13	a	74.68	0.28231	YES	YES
14	a	78.64	0.28640	YES	YES
15	a	86.87	0.22244	YES	YES
16	a	92.50	0.63221	YES	YES
17	a	95.52	1.22483	YES	YES
18	a	100.13	0.02259	YES	YES
19	a	110.64	1.46995	YES	YES
20	a	134.65	0.58483	YES	YES
21	a	154.92	1.77198	YES	YES
22	a	168.01	0.43068	YES	YES
23	a	191.21	2.88992	YES	YES
24	a	204.06	0.04844	YES	YES
25	a	218.20	1.83517	YES	YES
26	a	245.89	0.16399	YES	YES
27	a	264.59	0.28702	YES	YES
28	a	281.62	1.29168	YES	YES
29	a	306.04	1.87473	YES	YES
30	a	320.05	2.46467	YES	YES
31	a	349.10	0.07857	YES	YES
32	a	357.62	0.91673	YES	YES
33	a	411.52	3.23641	YES	YES
34	a	413.58	0.11381	YES	YES
35	a	433.61	2.99339	YES	YES
36	a	453.82	0.36253	YES	YES
37	a	458.11	0.55712	YES	YES
38	a	465.67	0.55181	YES	YES
39	a	475.22	1.37219	YES	YES
40	a	489.37	4.35182	YES	YES
41	a	505.21	4.77785	YES	YES
42	a	515.59	11.10122	YES	YES
43	a	519.17	12.44789	YES	YES
44	a	530.62	5.92420	YES	YES
45	a	540.35	11.68463	YES	YES
46	a	545.26	3.48926	YES	YES
47	a	563.04	5.39888	YES	YES
48	a	606.72	24.11151	YES	YES
49	a	615.07	18.59324	YES	YES
50	a	622.05	7.04463	YES	YES

3bf

SCF Energy (au) BP86/SV(P) -2376.715791997
SCF Energy (au) PBE0/def2-TZVPP -2376.297634233
SCF Energy (au) PBE0/def2-TZVPP -2376.3055857295 (Toluene Correction)
Zero Point Energy (au) 0.2836993
Chemical Potential (kJ mol^{-1}) 598.37
Dispersion Correction (au)PBE0/def2-TZVPP -0.06503775

xyz coordinates
41

Mn	1.2193489	0.6020264	0.8606017
C	1.6842037	0.8796677	2.6111754
C	2.8635536	0.0347297	0.3892382
C	1.6136558	2.2512375	0.4220448
O	1.8430488	3.3662344	0.1421678
O	3.9243350	-0.3226417	0.0636773
O	2.0099078	1.0716719	3.7144017
C	-1.3157925	-0.2381116	1.6367694
C	-1.5220768	2.0153745	1.0217826
C	-2.8892199	2.0182225	1.3273910
C	-3.4786214	0.8418555	1.8179138
C	-2.6790387	-0.3019325	1.9735991
C	-0.3847977	-1.3973172	1.7667139
C	0.2782322	-1.9556667	0.6205201
C	1.0105745	-3.1603577	0.8100076
C	1.1196397	-3.7711764	2.0612806
C	0.4856663	-3.2003028	3.1849117
C	-0.2675173	-2.0340653	3.0299354
H	-1.0102054	2.9143696	0.6432601
H	-3.4772754	2.9376370	1.1816374
H	-4.5511404	0.8118623	2.0692392
H	-3.1011012	-1.2513266	2.3378737
H	1.5021338	-3.6107959	-0.0682391
H	1.7046006	-4.6994786	2.1693927
H	0.5748327	-3.6726192	4.1765020
H	-0.7836713	-1.5916614	3.8981051
N	-0.7566698	0.9154196	1.1849338
C	0.4638524	0.5641322	-2.2739335
C	1.4741388	1.4300413	-2.7659224
C	1.3859130	2.0136955	-4.0373997
C	0.2610546	1.7505013	-4.8313512
C	-0.7687117	0.9135563	-4.3806572
C	-0.6592671	0.3264455	-3.1124551
H	2.3588837	1.6352477	-2.1437123
H	2.1767868	2.6771795	-4.4209382
F	0.1600023	2.3228520	-6.0494858
H	-1.6444173	0.7381501	-5.0252582
H	-1.4724362	-0.3201573	-2.7445602
C	0.5544993	-0.0746596	-0.9524162
C	0.1756649	-1.3671346	-0.7406668
H	-0.0825691	-2.0627050	-1.5680801

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	26.77	0.20929	YES	YES

8	a	35.17	0.34218	YES	YES
9	a	43.76	0.07449	YES	YES
10	a	51.77	0.04781	YES	YES
11	a	56.52	0.02224	YES	YES
12	a	65.03	0.45307	YES	YES
13	a	75.62	0.26948	YES	YES
14	a	85.39	0.07668	YES	YES
15	a	94.89	1.43426	YES	YES
16	a	99.61	0.91990	YES	YES
17	a	104.50	0.18700	YES	YES
18	a	107.39	0.10932	YES	YES
19	a	139.09	0.09849	YES	YES
20	a	144.26	0.18890	YES	YES
21	a	160.21	1.62454	YES	YES
22	a	191.69	1.00490	YES	YES
23	a	214.21	1.03482	YES	YES
24	a	232.05	0.45241	YES	YES
25	a	285.99	2.11397	YES	YES
26	a	294.17	1.63832	YES	YES
27	a	303.39	2.14950	YES	YES
28	a	353.23	0.16027	YES	YES
29	a	365.44	1.32245	YES	YES
30	a	401.71	4.96093	YES	YES
31	a	416.92	0.44825	YES	YES
32	a	425.01	1.63155	YES	YES
33	a	443.83	0.90585	YES	YES
34	a	457.88	0.43720	YES	YES
35	a	459.00	0.25517	YES	YES
36	a	476.86	0.88823	YES	YES
37	a	479.54	4.53331	YES	YES
38	a	488.56	0.74087	YES	YES
39	a	503.99	5.66997	YES	YES
40	a	505.86	8.85895	YES	YES
41	a	520.33	11.79803	YES	YES
42	a	537.67	2.67685	YES	YES
43	a	541.17	10.51813	YES	YES
44	a	552.49	0.41224	YES	YES
45	a	558.84	0.56721	YES	YES
46	a	604.48	10.51765	YES	YES
47	a	622.15	39.45123	YES	YES
48	a	622.69	5.24592	YES	YES
49	a	628.44	20.32636	YES	YES
50	a	633.02	19.60220	YES	YES

3bf'

SCF Energy (au) BP86/SV(P) -2376.712862759
SCF Energy (au) PBE0/def2-TZVPP -2376.295538110
SCF Energy (au) PBE0/def2-TZVPP -2376.3037174351 (Toluene Correction)
Zero Point Energy (au) 0.2837056
Chemical Potential (kJ mol^{-1}) 597.71
Dispersion Correction (au) PBE0/def2-TZVPP -0.06440518

xyz coordinates
41

Mn	1.4841279	1.7117603	0.8161645
C	1.8347473	2.1095485	2.5732290
C	3.1379523	1.0696979	0.5072899
C	1.9390421	3.3004134	0.2278432
O	2.2002880	4.3615391	-0.1939786
O	4.2031005	0.6530320	0.2834789
O	2.0980604	2.3800517	3.6768443
C	-1.0912426	0.8955884	1.3618890
C	-1.2679949	3.1650984	0.8042767
C	-2.6571279	3.1446433	0.9918775
C	-3.2723958	1.9467289	1.3888197
C	-2.4757778	0.8045197	1.5771501
C	-0.1360325	-0.2393286	1.5618573
C	0.5855734	-0.8182385	0.4659734
C	1.3878778	-1.9607722	0.7345586
C	1.4896605	-2.5042610	2.0172579
C	0.7777799	-1.9268438	3.0901668
C	-0.0303131	-0.8122031	2.8587612
H	-0.7343996	4.0804218	0.5014531
H	-3.2424425	4.0630071	0.8290436
H	-4.3620244	1.8993039	1.5462304
H	-2.9154253	-0.1586595	1.8792875
H	1.9362159	-2.4188131	-0.1045801
H	2.1299847	-3.3849637	2.1900484
H	0.8566168	-2.3503587	4.1044705
H	-0.5971524	-0.3585124	3.6884911
N	-0.5095354	2.0666317	0.9942040
H	1.0145027	1.5569886	-1.9830248
C	0.9763957	1.0270270	-1.0116645
C	0.5225045	-0.2547710	-0.9302930
C	0.0619967	-1.1225549	-2.0449167
C	-0.8527700	-2.7478115	-4.1697179
C	-1.2287016	-3.0580846	-2.8570813
C	-0.7701515	-2.2457407	-1.8084125
C	0.4233886	-0.8492925	-3.3891059
C	-0.0298422	-1.6463722	-4.4476822
F	-1.2820083	-3.5260240	-5.1857821
H	-1.8773332	-3.9283335	-2.6700729
H	-1.0765659	-2.4870338	-0.7772746
H	1.0912536	-0.0008119	-3.6073525
H	0.2581675	-1.4362164	-5.4897271

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	24.62	0.36777	YES	YES

8	a	34.24	0.13052	YES	YES
9	a	40.74	0.50128	YES	YES
10	a	52.69	0.03101	YES	YES
11	a	53.24	0.17478	YES	YES
12	a	71.92	1.11648	YES	YES
13	a	76.77	0.25782	YES	YES
14	a	83.21	0.23343	YES	YES
15	a	89.53	0.46304	YES	YES
16	a	93.28	0.18580	YES	YES
17	a	97.80	0.77714	YES	YES
18	a	103.60	0.00812	YES	YES
19	a	137.41	1.20567	YES	YES
20	a	153.58	0.57525	YES	YES
21	a	171.04	1.05843	YES	YES
22	a	203.77	0.97908	YES	YES
23	a	207.67	0.08842	YES	YES
24	a	243.63	0.46889	YES	YES
25	a	260.86	0.45042	YES	YES
26	a	303.88	1.62775	YES	YES
27	a	320.42	1.57653	YES	YES
28	a	340.64	0.35798	YES	YES
29	a	357.53	0.88841	YES	YES
30	a	395.13	2.68512	YES	YES
31	a	412.39	0.02398	YES	YES
32	a	424.94	0.63912	YES	YES
33	a	435.67	3.16904	YES	YES
34	a	457.09	0.86556	YES	YES
35	a	462.47	0.17062	YES	YES
36	a	475.11	1.19513	YES	YES
37	a	487.90	3.87155	YES	YES
38	a	496.79	17.14149	YES	YES
39	a	503.35	5.61634	YES	YES
40	a	517.87	11.40446	YES	YES
41	a	525.85	8.38907	YES	YES
42	a	536.67	2.63981	YES	YES
43	a	544.98	3.90885	YES	YES
44	a	563.85	6.90296	YES	YES
45	a	605.97	20.59872	YES	YES
46	a	615.23	21.57449	YES	YES
47	a	622.45	6.64940	YES	YES
48	a	624.34	31.15951	YES	YES
49	a	631.27	3.33761	YES	YES
50	a	635.77	17.39122	YES	YES

3bg

SCF Energy (au) BP86/SV(P) -2614.359816251
SCF Energy (au) PBE0/def2-TZVPP -2613.984795259
SCF Energy (au) PBE0/def2-TZVPP -2613.9929371345 (Toluene Correction)
Zero Point Energy (au) 0.2962443
Chemical Potential (kJ mol^{-1}) 619.21
Dispersion Correction (au) PBE0/def2-TZVPP -0.06852295

xyz coordinates
44

Mn	1.1861921	0.4233087	1.3165635
C	1.6496781	0.7318831	3.0615198
C	2.8324442	-0.1503251	0.8592402
C	1.5764145	2.0672875	0.8494133
O	1.8015756	3.1767450	0.5480063
O	3.8942168	-0.5116914	0.5419882
O	1.9743651	0.9448360	4.1608879
C	-1.3359910	-0.4259872	2.0901301
C	-1.5663266	1.8264098	1.4793153
C	-2.9334150	1.8137320	1.7861338
C	-3.5094618	0.6301670	2.2749196
C	-2.6977821	-0.5057507	2.4280755
C	-0.3888597	-1.5738836	2.2204790
C	0.2601682	-2.1423136	1.0719082
C	1.0035837	-3.3393906	1.2618963
C	1.1376889	-3.9335189	2.5188968
C	0.5185693	-3.3527583	3.6456958
C	-0.2463025	-2.1944069	3.4895463
H	-1.0640941	2.7313999	1.1019798
H	-3.5317034	2.7268438	1.6427157
H	-4.5812509	0.5884699	2.5276280
H	-3.1091275	-1.4598707	2.7922637
H	1.4842035	-3.7967404	0.3812146
H	1.7309746	-4.8562239	2.6289410
H	0.6280887	-3.8119997	4.6413336
H	-0.7523739	-1.7459878	4.3605277
N	-0.7901591	0.7339893	1.6397458
C	0.4502444	0.3771908	-1.8134071
C	1.5031279	1.1820141	-2.3181999
C	1.4211083	1.7775904	-3.5819796
C	0.2699348	1.6042905	-4.3750452
C	-0.7943677	0.8213249	-3.8886097
C	-0.7019962	0.2157855	-2.6292994
H	2.4086376	1.3296299	-1.7098435
H	2.2543302	2.3941246	-3.9533462
C	0.1970226	2.2168518	-5.7520544
H	-1.7037872	0.6935105	-4.4967259
H	-1.5460078	-0.3813972	-2.2477264
C	0.5271147	-0.2669150	-0.4950082
C	0.1438119	-1.5578492	-0.2905013
H	-0.1236005	-2.2496742	-1.1179296
F	0.9269758	3.3565088	-5.8407486
F	-1.0778491	2.5221585	-6.1055511
F	0.6739844	1.3706320	-6.7049893

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	21.16	0.19647	YES	YES
8	a	30.62	0.37460	YES	YES
9	a	34.38	0.08761	YES	YES
10	a	43.31	0.02830	YES	YES
11	a	45.44	0.00144	YES	YES
12	a	52.76	0.09202	YES	YES
13	a	61.15	0.48361	YES	YES
14	a	76.48	0.23164	YES	YES
15	a	85.17	0.06903	YES	YES
16	a	89.14	0.08270	YES	YES
17	a	94.28	1.18713	YES	YES
18	a	97.77	0.86356	YES	YES
19	a	105.08	0.11509	YES	YES
20	a	115.00	0.60942	YES	YES
21	a	124.46	0.08990	YES	YES
22	a	142.91	1.09096	YES	YES
23	a	165.52	0.91736	YES	YES
24	a	193.41	1.03521	YES	YES
25	a	206.99	1.04327	YES	YES
26	a	209.37	0.23505	YES	YES
27	a	246.59	0.58105	YES	YES
28	a	289.94	0.90528	YES	YES
29	a	302.57	1.09223	YES	YES
30	a	311.33	4.35150	YES	YES
31	a	353.49	1.33456	YES	YES
32	a	365.35	0.63782	YES	YES
33	a	388.01	1.67649	YES	YES
34	a	403.34	2.38918	YES	YES
35	a	406.95	2.43588	YES	YES
36	a	423.41	3.80656	YES	YES
37	a	443.59	2.53152	YES	YES
38	a	455.39	0.11763	YES	YES
39	a	459.59	0.25725	YES	YES
40	a	476.40	0.49494	YES	YES
41	a	480.99	4.10822	YES	YES
42	a	492.52	2.78660	YES	YES
43	a	505.99	5.85205	YES	YES
44	a	506.58	9.33807	YES	YES
45	a	528.92	2.64916	YES	YES
46	a	535.96	1.06907	YES	YES
47	a	549.17	2.80493	YES	YES
48	a	552.38	1.11732	YES	YES
49	a	568.97	0.13806	YES	YES
50	a	576.26	6.76105	YES	YES

3bg'

SCF Energy (au) BP86/SV(P) -2614.357206437
SCF Energy (au) PBE0/def2-TZVPP -2613.982644347
SCF Energy (au) PBE0/def2-TZVPP -2613.9909778406 (Toluene Correction)
Zero Point Energy (au) 0.2962383
Chemical Potential (kJ mol^{-1}) 618.34
Dispersion Correction (au) PBE0/def2-TZVPP -0.06781524

xyz coordinates
44

Mn	1.6001682	1.9660958	1.2084954
C	1.9402133	2.3601237	2.9702089
C	3.2552590	1.3172544	0.9168275
C	2.0678143	3.5539099	0.6260754
O	2.3383040	4.6136584	0.2077755
O	4.3208450	0.8957304	0.7063910
O	2.1966241	2.6283642	4.0754364
C	-0.9835461	1.1633802	1.7461958
C	-1.1452378	3.4336904	1.1871035
C	-2.5350874	3.4209000	1.3699921
C	-3.1584688	2.2264742	1.7648863
C	-2.3692137	1.0798174	1.9566628
C	-0.0337177	0.0245597	1.9488109
C	0.6938366	-0.5506656	0.8554690
C	1.5003815	-1.6897805	1.1248842
C	1.5970839	-2.2362874	2.4068790
C	0.8769778	-1.6642491	3.4769506
C	0.0669285	-0.5510369	3.2447207
H	-0.6057135	4.3459505	0.8855869
H	-3.1147598	4.3424036	1.2049079
H	-4.2489407	2.1851419	1.9179131
H	-2.8155056	0.1192388	2.2572971
H	2.0553274	-2.1439724	0.2879564
H	2.2393663	-3.1152472	2.5808171
H	0.9515830	-2.0904000	4.4904534
H	-0.5043819	-0.1005059	4.0730469
N	-0.3937996	2.3309129	1.3799587
H	1.1424550	1.8252016	-1.5900900
C	1.1010036	1.2923378	-0.6205604
C	0.6327642	0.0146024	-0.5412096
C	0.1520765	-0.8394015	-1.6544086
C	-0.8006482	-2.4659841	-3.7918210
C	-1.1247657	-2.7817152	-2.4594137
C	-0.6540416	-1.9806723	-1.4108200
C	0.4642913	-0.5384421	-3.0052720
C	-0.0045216	-1.3329374	-4.0560291
C	-1.2384704	-3.3710109	-4.9169275
H	-1.7555102	-3.6578757	-2.2413575
H	-0.9280730	-2.2405682	-0.3753446
H	1.1037146	0.3290837	-3.2325959
H	0.2560351	-1.0779295	-5.0951339
F	-0.3354706	-4.3639575	-5.1412764
F	-1.3787107	-2.6995453	-6.0876251
F	-2.4244684	-3.9766473	-4.6518171

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.68	0.52294	YES	YES
8	a	26.46	0.13913	YES	YES
9	a	32.03	0.26819	YES	YES
10	a	41.65	0.40771	YES	YES
11	a	48.83	0.05953	YES	YES
12	a	53.68	0.29348	YES	YES
13	a	63.35	1.14071	YES	YES
14	a	73.77	0.06558	YES	YES
15	a	77.85	0.22656	YES	YES
16	a	84.33	0.31054	YES	YES
17	a	91.53	0.39077	YES	YES
18	a	95.57	0.57094	YES	YES
19	a	99.41	0.23112	YES	YES
20	a	120.35	1.01401	YES	YES
21	a	132.15	0.20509	YES	YES
22	a	159.95	0.84835	YES	YES
23	a	171.94	1.33900	YES	YES
24	a	186.84	0.47245	YES	YES
25	a	195.29	0.80549	YES	YES
26	a	221.48	0.38611	YES	YES
27	a	263.02	1.98195	YES	YES
28	a	267.54	0.28038	YES	YES
29	a	301.13	0.31184	YES	YES
30	a	323.00	3.63535	YES	YES
31	a	348.55	0.80659	YES	YES
32	a	361.83	2.92247	YES	YES
33	a	382.91	0.74989	YES	YES
34	a	397.60	2.23162	YES	YES
35	a	404.48	1.12542	YES	YES
36	a	432.96	8.21703	YES	YES
37	a	436.02	5.05123	YES	YES
38	a	458.17	3.76486	YES	YES
39	a	461.98	3.13311	YES	YES
40	a	474.49	1.24921	YES	YES
41	a	482.14	4.98839	YES	YES
42	a	491.52	1.26753	YES	YES
43	a	515.90	6.81848	YES	YES
44	a	521.01	9.17935	YES	YES
45	a	531.91	0.61700	YES	YES
46	a	543.89	4.41968	YES	YES
47	a	555.20	2.97278	YES	YES
48	a	565.14	1.58730	YES	YES
49	a	577.77	1.37054	YES	YES
50	a	593.16	2.46991	YES	YES

3bh

SCF Energy (au) BP86/SV(P)	-2505.273702407
SCF Energy (au) PBE0/def2-TZVPP	-2504.831435415
SCF Energy (au) PBE0/def2-TZVPP	-2504.8417586438 (Toluene Correction)
Zero Point Energy (au)	0.3330534
Chemical Potential (kJ mol^{-1})	713.51
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07112017

xyz coordinates
47

Mn	1.1127105	0.1658704	1.8333390
C	1.5835667	0.4652460	3.5777114
C	2.7580751	-0.4013803	1.3658922
C	1.4987726	1.8125468	1.3726203
O	1.7223402	2.9241475	1.0778646
O	3.8197636	-0.7593539	1.0442834
O	1.9126438	0.6717683	4.6772089
C	-1.4083933	-0.6864908	2.6225665
C	-1.6393087	1.5654795	2.0113434
C	-3.0045365	1.5549963	2.3260552
C	-3.5795623	0.3725487	2.8187640
C	-2.7685323	-0.7641869	2.9680342
C	-0.4628153	-1.8353476	2.7491352
C	0.1903774	-2.3969144	1.5994388
C	0.9370427	-3.5926930	1.7871187
C	1.0689458	-4.1922977	3.0417279
C	0.4441777	-3.6187550	4.1690795
C	-0.3227804	-2.4613801	4.0156019
H	-1.1382390	2.4694458	1.6301879
H	-3.6023673	2.4687759	2.1851321
H	-4.6500949	0.3322759	3.0769977
H	-3.1792429	-1.7176700	3.3346265
H	1.4210940	-4.0452573	0.9058355
H	1.6643287	-5.1139616	3.1493900
H	0.5510143	-4.0825979	5.1629201
H	-0.8324425	-2.0179584	4.8870611
N	-0.8633106	0.4723700	2.1681784
C	0.3546108	0.1156761	-1.2967836
C	1.3937879	0.9355107	-1.8095598
C	1.3014148	1.5180366	-3.0781817
C	0.1508371	1.3199446	-3.8747206
C	-0.8979050	0.5181877	-3.3735738
C	-0.7967238	-0.0741491	-2.1113860
H	2.2977957	1.0998998	-1.2026855
H	2.1238572	2.1399783	-3.4621786
C	-0.0148038	1.9274728	-5.2272940
H	-1.7927646	0.3752723	-3.9999790
H	-1.6273941	-0.6863229	-1.7237034
C	0.4438958	-0.5211862	0.0233078
C	0.0692481	-1.8140045	0.2365671
H	-0.1943918	-2.5108049	-0.5878937
O	1.0685248	2.6674624	-5.5973594
O	-0.9976746	1.7912167	-5.9403573
C	0.9803481	3.2813351	-6.8872879
H	1.9278126	3.8392272	-7.0223537
H	0.1117819	3.9733183	-6.9386616
H	0.8645159	2.5147030	-7.6840296

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	21.47	0.25461	YES	YES
8	a	29.01	0.98577	YES	YES
9	a	36.31	1.24804	YES	YES
10	a	43.19	0.04438	YES	YES
11	a	49.37	0.17824	YES	YES
12	a	60.58	0.47438	YES	YES
13	a	72.51	0.60654	YES	YES
14	a	76.70	0.17487	YES	YES
15	a	83.77	0.35492	YES	YES
16	a	85.91	0.04484	YES	YES
17	a	94.45	1.25210	YES	YES
18	a	96.61	0.86233	YES	YES
19	a	104.33	0.04465	YES	YES
20	a	110.46	0.11004	YES	YES
21	a	116.69	0.76729	YES	YES
22	a	122.66	0.49100	YES	YES
23	a	145.17	0.74573	YES	YES
24	a	155.67	0.42430	YES	YES
25	a	165.40	1.94312	YES	YES
26	a	196.82	0.30048	YES	YES
27	a	202.74	2.62503	YES	YES
28	a	231.80	0.93245	YES	YES
29	a	265.95	4.40239	YES	YES
30	a	291.06	0.35258	YES	YES
31	a	300.26	8.23611	YES	YES
32	a	319.46	10.79951	YES	YES
33	a	335.23	2.25638	YES	YES
34	a	360.78	1.49515	YES	YES
35	a	397.04	0.64580	YES	YES
36	a	410.01	0.38725	YES	YES
37	a	415.09	1.68924	YES	YES
38	a	434.16	1.71597	YES	YES
39	a	448.98	0.27168	YES	YES
40	a	458.05	0.85427	YES	YES
41	a	471.42	3.20674	YES	YES
42	a	476.46	0.29819	YES	YES
43	a	483.71	5.55441	YES	YES
44	a	493.53	4.04021	YES	YES
45	a	507.03	9.25964	YES	YES
46	a	509.77	7.06654	YES	YES
47	a	536.07	0.97439	YES	YES
48	a	541.46	5.73429	YES	YES
49	a	550.95	1.47145	YES	YES
50	a	560.15	1.29427	YES	YES
51	a	581.11	3.81664	YES	YES

3bh'

SCF Energy (au) BP86/SV(P)		-2505.271309102
SCF Energy (au) PBE0/def2-TZVPP		-2504.829599821
SCF Energy (au) PBE0/def2-TZVPP		-2504.8400771336 (Toluene Correction)
Zero Point Energy (au)		0.3330903
Chemical Potential (kJ mol^{-1})		712.91
Dispersion Correction (au)	PBE0/def2-TZVPP	-0.07050338

xyz coordinates

47

Mn	1.6951515	2.2430586	1.7176277
C	2.0101655	2.6557657	3.4800857
C	3.3595998	1.6083577	1.4508410
C	2.1535237	3.8297089	1.1245673
O	2.4173128	4.8883301	0.6988351
O	4.4319548	1.1965283	1.2556827
O	2.2528970	2.9349053	4.5857533
C	-0.8911553	1.4255255	2.2317931
C	-1.0636848	3.6857983	1.6372204
C	-2.4562428	3.6626635	1.7969004
C	-3.0754853	2.4682106	2.1983456
C	-2.2793436	1.3318583	2.4201525
C	0.0665331	0.2994706	2.4640724
C	0.8181627	-0.2785311	1.3889900
C	1.6377436	-1.4017069	1.6847080
C	1.7222910	-1.9311725	2.9746488
C	0.9762750	-1.3577444	4.0261294
C	0.1542544	-0.2591693	3.7681922
H	-0.5275454	4.5985734	1.3312333
H	-3.0414274	4.5761381	1.6082466
H	-4.1680748	2.4187907	2.3328839
H	-2.7219556	0.3712217	2.7259262
H	2.2111109	-1.8581712	0.8615820
H	2.3743136	-2.7985375	3.1693147
H	1.0405027	-1.7712958	5.0455614
H	-0.4361572	0.1931152	4.5820178
N	-0.3055626	2.5929144	1.8583711
H	1.2733847	2.0659007	-1.0847791
C	1.2260194	1.5444683	-0.1094272
C	0.7639596	0.2647934	-0.0173071
C	0.2863037	-0.6035700	-1.1187124
C	-0.6827035	-2.2508569	-3.2398217
C	-0.9766216	-2.5633958	-1.8956706
C	-0.5001765	-1.7566044	-0.8571930
C	0.5785651	-0.3053822	-2.4761989
C	0.1032394	-1.1077699	-3.5164954
C	-1.2145995	-3.1489235	-4.3044051
H	-1.5907120	-3.4538243	-1.6870042
H	-0.7510834	-2.0168623	0.1842040
H	1.2080316	0.5669184	-2.7138496
H	0.3471571	-0.8613470	-4.5608105
O	-0.8560241	-2.7367563	-5.5540155
O	-1.8957086	-4.1438773	-4.1059219
C	-1.3314246	-3.5532820	-6.6293140
H	-2.4423585	-3.5923027	-6.6363219
H	-0.9454243	-4.5917947	-6.5390658
H	-0.9549812	-3.0801377	-7.5575728

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.32	0.40677	YES	YES
8	a	30.33	0.77351	YES	YES
9	a	33.68	1.59592	YES	YES
10	a	45.15	0.07589	YES	YES
11	a	52.02	0.21572	YES	YES
12	a	61.41	0.36558	YES	YES
13	a	69.80	2.06162	YES	YES
14	a	73.43	0.09241	YES	YES
15	a	79.52	0.14497	YES	YES
16	a	84.06	0.11968	YES	YES
17	a	91.95	0.36492	YES	YES
18	a	95.46	0.71358	YES	YES
19	a	98.89	0.16745	YES	YES
20	a	112.27	0.74477	YES	YES
21	a	119.97	0.79742	YES	YES
22	a	124.94	0.35669	YES	YES
23	a	152.47	0.60793	YES	YES
24	a	161.11	2.48913	YES	YES
25	a	169.65	0.53274	YES	YES
26	a	192.71	1.55445	YES	YES
27	a	205.35	0.68783	YES	YES
28	a	252.07	1.34069	YES	YES
29	a	257.35	1.83314	YES	YES
30	a	282.23	2.78482	YES	YES
31	a	304.70	1.73210	YES	YES
32	a	315.40	14.71030	YES	YES
33	a	335.86	5.17570	YES	YES
34	a	354.76	1.22162	YES	YES
35	a	369.92	0.72028	YES	YES
36	a	408.22	0.34369	YES	YES
37	a	431.27	5.32783	YES	YES
38	a	438.07	5.17158	YES	YES
39	a	456.80	1.67779	YES	YES
40	a	461.73	5.07869	YES	YES
41	a	474.36	1.72360	YES	YES
42	a	478.04	4.53376	YES	YES
43	a	478.84	3.91006	YES	YES
44	a	492.21	2.50350	YES	YES
45	a	516.49	8.45721	YES	YES
46	a	521.47	8.82860	YES	YES
47	a	532.75	0.54265	YES	YES
48	a	544.48	4.99197	YES	YES
49	a	561.64	3.10440	YES	YES
50	a	598.51	1.83620	YES	YES

3bi

SCF Energy (au) BP86/SV(P)	-2508.437513184
SCF Energy (au) PBE0/def2-TZVPP	-2507.961431247
SCF Energy (au) PBE0/def2-TZVPP	-2507.9706202452 (Toluene Correction)
Zero Point Energy (au)	0.3703473
Chemical Potential (kJ mol^{-1})	811.94
Dispersion Correction (au) PBE0/def2-TZVPP	-0.08161133

xyz coordinates
51

Mn	1.3161635	1.1650105	1.4833797
C	1.6593210	1.4842760	3.2533358
C	2.9754658	0.5498513	1.1511691
C	1.7828870	2.7957704	1.0178426
O	2.0615356	3.8928395	0.7197043
O	4.0508324	0.1662239	0.9123884
O	1.9147016	1.7039945	4.3703257
C	-1.2654764	0.4009478	2.0629745
C	-1.4245780	2.6380882	1.3808562
C	-2.8135249	2.6368021	1.5736835
C	-3.4361283	1.4687205	2.0420246
C	-2.6486650	0.3311229	2.2903335
C	-0.3040279	-0.7176535	2.2948607
C	0.4669182	-1.2705477	1.2171751
C	1.3111559	-2.3784035	1.5152922
C	1.4018540	-2.9126801	2.8009692
C	0.6286248	-2.3680511	3.8499410
C	-0.2175971	-1.2889934	3.5942423
H	-0.8858776	3.5305258	1.0244945
H	-3.3930862	3.5481466	1.3592108
H	-4.5253477	1.4398180	2.2066012
H	-3.0952519	-0.6107349	2.6451183
H	1.8933520	-2.8203291	0.6906032
H	2.0741194	-3.7644823	2.9952703
H	0.6930241	-2.7894471	4.8662471
H	-0.8236213	-0.8558833	4.4069113
N	-0.6742083	1.5465764	1.6342579
C	0.7019729	1.2990344	-1.6199975
C	1.8435003	1.9545775	-2.1486610
C	1.7585213	2.7274754	-3.3162998
C	0.5255875	2.8925712	-3.9729487
C	-0.6211451	2.2676907	-3.4516204
C	-0.5348133	1.4762490	-2.2960780
H	2.8126037	1.8416152	-1.6360318
H	2.6650371	3.2152519	-3.7125717
H	0.4580007	3.5111171	-4.8832601
H	-1.5954982	2.3933875	-3.9537007
H	-1.4352166	0.9794639	-1.8993542
C	0.7706214	0.5081032	-0.3822832
C	0.3582104	-0.7845400	-0.2063863
C	-0.0842868	-1.7713981	-1.2312206
C	-0.9525822	-3.6806862	-3.1567423
C	-1.4574443	-3.7174792	-1.8456476
C	-1.0252052	-2.7783581	-0.8960580
C	0.4245111	-1.7590372	-2.5546917
C	-0.0064244	-2.6984375	-3.5026079
H	-1.2879851	-4.4186849	-3.9042361
H	-2.1964495	-4.4845197	-1.5584149
H	-1.4334390	-2.8176048	0.1279640
H	1.1795737	-1.0088331	-2.8347555
H	0.4097852	-2.6684663	-4.5236090

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	25.86	0.09436	YES	YES
8	a	29.50	0.18490	YES	YES
9	a	40.32	0.30306	YES	YES
10	a	41.33	0.44143	YES	YES
11	a	52.94	0.08549	YES	YES
12	a	54.89	0.03200	YES	YES
13	a	59.74	0.25229	YES	YES
14	a	68.71	0.07958	YES	YES
15	a	77.02	1.14270	YES	YES
16	a	82.37	0.69631	YES	YES
17	a	86.47	0.49161	YES	YES
18	a	95.32	0.27536	YES	YES
19	a	97.69	0.57342	YES	YES
20	a	104.79	0.29736	YES	YES
21	a	108.64	0.81777	YES	YES
22	a	145.85	0.50143	YES	YES
23	a	161.14	0.79578	YES	YES
24	a	176.47	0.59376	YES	YES
25	a	190.30	0.24471	YES	YES
26	a	213.84	0.19749	YES	YES
27	a	222.98	0.33355	YES	YES
28	a	229.16	0.75418	YES	YES
29	a	250.61	0.27012	YES	YES
30	a	262.46	0.46384	YES	YES
31	a	322.56	0.72430	YES	YES
32	a	331.75	1.46288	YES	YES
33	a	362.43	0.29753	YES	YES
34	a	402.26	0.16382	YES	YES
35	a	405.84	0.12806	YES	YES
36	a	423.68	4.33802	YES	YES
37	a	440.44	1.56353	YES	YES
38	a	446.26	0.33748	YES	YES
39	a	456.75	2.33162	YES	YES
40	a	462.56	0.15073	YES	YES
41	a	478.00	0.30726	YES	YES
42	a	484.74	4.15259	YES	YES
43	a	494.31	0.50231	YES	YES
44	a	508.46	6.46553	YES	YES
45	a	517.55	3.38325	YES	YES
46	a	532.07	3.93291	YES	YES
47	a	540.44	7.63454	YES	YES
48	a	550.21	2.02811	YES	YES
49	a	571.73	3.60312	YES	YES
50	a	584.40	11.80876	YES	YES

3bj

SCF Energy (au) BP86/SV(P)	-2360.901282159
SCF Energy (au) PBE0/def2-TZVPP	-2360.472310505
SCF Energy (au) PBE0/def2-TZVPP	-2360.4790774360 (Toluene Correction)
Zero Point Energy (au)	0.4322002
Chemical Potential (kJ mol^{-1})	964.24
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07607291

xyz coordinates

55

Mn	1.1113667	1.3348724	1.5861612
C	1.4699877	1.6516653	3.3555589
C	2.8218391	0.9509411	1.1861731
C	1.3330937	3.0123303	1.1264244
O	1.4398562	4.1363383	0.8073253
O	3.9285700	0.7046753	0.9101342
O	1.7404877	1.8868693	4.4664707
C	-1.3153556	0.1806963	2.1987127
C	-1.8014961	2.4149834	1.6870746
C	-3.1674101	2.2149889	1.9303737
C	-3.6086731	0.9444533	2.3338820
C	-2.6660703	-0.0889149	2.4701893
C	-0.2103162	-0.8145822	2.3344299
C	0.5835278	-1.2038861	1.2030727
C	1.5696859	-2.2093300	1.4160756
C	1.7680680	-2.8008236	2.6650358
C	0.9733459	-2.4150911	3.7657916
C	-0.0059727	-1.4356985	3.5963081
H	-1.4013997	3.3956176	1.3832849
H	-3.8705058	3.0535141	1.8076860
H	-4.6756997	0.7575646	2.5365705
H	-2.9662670	-1.1038212	2.7735359
H	2.1907749	-2.5199581	0.5601292
H	2.5487827	-3.5692345	2.7908357
H	1.1263528	-2.8784258	4.7539492
H	-0.6310610	-1.1247324	4.4495925
N	-0.9007362	1.4207614	1.8281105
C	0.5340973	1.4830152	-1.5717078
C	0.6101608	0.6849800	-0.2971277
C	0.3643061	-0.6474948	-0.1797845
C	-0.0538543	-1.6305026	-1.2656334
C	1.9156541	1.8340703	-2.1693745
H	-0.0592331	0.9432910	-2.3499352
H	-0.0129976	2.4375429	-1.3802344
H	0.6437644	-2.5030730	-1.2694781
H	0.0528994	-1.1530217	-2.2640702
C	-1.4947183	-2.1614023	-1.1072581
C	-1.8910644	-3.1959064	-2.1738244
H	-2.2024189	-1.2998908	-1.1401389
H	-1.6118991	-2.6166206	-0.0945834
H	-1.1802749	-4.0550810	-2.1326536
H	-1.7624382	-2.7453962	-3.1863849
C	-3.3279942	-3.7127451	-2.0228591
H	-3.5784653	-4.4590346	-2.8089909
H	-4.0672098	-2.8831574	-2.1005283
H	-3.4804237	-4.2028354	-1.0343510
H	2.5166168	2.3866163	-1.4115243
C	1.8301680	2.6701349	-3.4563536
H	2.4734648	0.8892167	-2.3710670
C	3.2025361	3.0100677	-4.0528118
H	1.2735884	3.6134453	-3.2424775
H	1.2206595	2.1220902	-4.2137046

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H     3.8228817    3.5909238   -3.3334414
H     3.1062444    3.6169160   -4.9805035
H     3.7711742    2.0880782   -4.3120859

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol         IR     RAMAN
     1                       0.00         0.00000       -       -
     2                       0.00         0.00000       -       -
     3                       0.00         0.00000       -       -
     4                       0.00         0.00000       -       -
     5                       0.00         0.00000       -       -
     6                       0.00         0.00000       -       -
     7        a             13.34         0.11283      YES     YES
     8        a             25.09         0.03129      YES     YES
     9        a             28.09         0.18786      YES     YES
    10        a             37.85         0.64049      YES     YES
    11        a             45.03         0.03562      YES     YES
    12        a             53.49         0.24346      YES     YES
    13        a             58.99         0.36465      YES     YES
    14        a             64.03         0.04008      YES     YES
    15        a             68.06         0.24588      YES     YES
    16        a             79.99         0.05926      YES     YES
    17        a             84.38         0.19486      YES     YES
    18        a             92.13         0.18692      YES     YES
    19        a             94.47         0.83761      YES     YES
    20        a             99.23         0.48696      YES     YES
    21        a            101.84         0.42884      YES     YES
    22        a            111.75         0.05655      YES     YES
    23        a            118.00         0.13203      YES     YES
    24        a            125.34         0.16412      YES     YES
    25        a            135.14         0.13516      YES     YES
    26        a            170.14         1.02048      YES     YES
    27        a            182.18         0.33801      YES     YES
    28        a            193.07         0.50594      YES     YES
    29        a            213.09         0.22804      YES     YES
    30        a            224.04         0.17526      YES     YES
    31        a            241.41         0.41886      YES     YES
    32        a            247.48         0.21790      YES     YES
    33        a            257.31         0.63362      YES     YES
    34        a            287.43         0.63535      YES     YES
    35        a            300.51         0.52641      YES     YES
    36        a            317.16         1.48427      YES     YES
    37        a            343.56         0.72950      YES     YES
    38        a            357.13         0.08179      YES     YES
    39        a            385.22         0.44102      YES     YES
    40        a            417.12         1.89289      YES     YES
    41        a            428.70         4.60147      YES     YES
    42        a            458.93         0.22510      YES     YES
    43        a            459.65         0.88291      YES     YES
    44        a            468.59         4.26916      YES     YES
    45        a            474.45         0.45687      YES     YES
    46        a            484.48         1.64184      YES     YES
    47        a            495.02         5.00263      YES     YES
    48        a            510.81         8.03576      YES     YES
    49        a            527.80         4.57164      YES     YES
    50        a            536.42         0.97409      YES     YES
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3ca

SCF Energy (au) BP86/SV(P) -2678.222750796
SCF Energy (au) PBE0/def2-TZVPP -2677.741199140
SCF Energy (au) PBE0/def2-TZVPP -2677.7536261288 (Toluene Correction)
Zero Point Energy (au) 0.4177735
Chemical Potential (kJ mol^{-1}) 922.06
Dispersion Correction (au) PBE0/def2-TZVPP -0.08529995

xyz coordinates
57

Mn	0.0636696	1.6111328	-0.8491924
C	1.5305880	2.1895400	0.0801886
C	1.0436225	0.5324623	-1.9059389
C	0.1688237	2.9320425	-2.0074271
O	0.2269811	3.8343760	-2.7520615
O	1.6792676	-0.1601746	-2.5968114
O	2.4830343	2.5639964	0.6417431
C	-1.4234957	1.7436940	1.4825916
C	-1.9635197	3.6789869	0.2797856
C	-2.8252705	4.1154596	1.2951276
C	-2.9710718	3.3305480	2.4511613
C	-2.2573617	2.1245152	2.5466824
C	-0.6267010	0.4849612	1.4533082
C	-0.8050618	-0.4633337	0.4197156
C	-0.1193440	-1.7697392	0.5270746
N	0.7698340	-1.9465157	1.6357918
C	0.9516228	-0.9885818	2.6165126
C	0.2530664	0.2037401	2.5436844
H	-1.8053058	4.2625049	-0.6407915
H	-3.3701369	5.0646763	1.1751830
H	-3.6377278	3.6509903	3.2679992
H	-2.3495205	1.4696870	3.4267453
O	-0.2933570	-2.6860680	-0.2787171
C	1.9011784	-1.2733206	3.7489853
H	0.4115791	0.9607065	3.3249413
N	-1.2724795	2.5243810	0.3818916
C	-2.5266545	0.9478085	-2.6966211
C	-2.0482630	1.4007388	-3.9528735
C	-2.9215011	1.6046010	-5.0314184
C	-4.3021051	1.3820062	-4.8814423
C	-4.7995416	0.9453821	-3.6404013
C	-3.9253567	0.7288513	-2.5653109
H	-0.9691196	1.5761126	-4.0850712
H	-2.5192581	1.9452965	-6.0002335
H	-4.9887656	1.5536703	-5.7270793
H	-5.8814529	0.7740495	-3.5079285
H	-4.3226241	0.3985879	-1.5910971
C	-1.6271725	0.7047443	-1.5632998
C	-1.7629983	-0.3443478	-0.7046295
H	-2.4346265	-1.2097105	-0.8829210
H	1.9823365	-0.3844132	4.4063731
H	2.9174770	-1.5269463	3.3760077
H	1.5564095	-2.1285800	4.3740081
C	1.4697500	-3.2492764	1.6847932
H	1.4258115	-3.6430046	2.7199194
C	2.9070780	-3.2156046	1.1879399
H	0.8632975	-3.9110563	1.0317846
C	5.5741048	-3.2363148	0.2415008
C	5.2677551	-3.7893264	1.4956591
C	3.9427165	-3.7747900	1.9648590
C	3.2231298	-2.6724219	-0.0763338
C	4.5476388	-2.6785393	-0.5415754

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H     6.6129593   -3.2415146   -0.1280164
H     6.0638343   -4.2325353    2.1167661
H     3.7094368   -4.2123280    2.9517072
H     2.4268794   -2.2536220   -0.7126693
H     4.7759111   -2.2481847   -1.5305696

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                        0.00         0.00000        -       -
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7        a              18.61         0.45792       YES     YES
     8        a              20.78         0.19310       YES     YES
     9        a              29.85         0.31391       YES     YES
    10        a              32.25         0.44016       YES     YES
    11        a              39.02         0.86850       YES     YES
    12        a              45.99         0.33234       YES     YES
    13        a              50.47         0.19399       YES     YES
    14        a              56.23         1.74737       YES     YES
    15        a              68.28         1.39703       YES     YES
    16        a              69.73         0.36509       YES     YES
    17        a              84.03         1.01838       YES     YES
    18        a              85.80         0.48941       YES     YES
    19        a              96.54         1.61114       YES     YES
    20        a              98.74         0.20719       YES     YES
    21        a             102.86         0.31583       YES     YES
    22        a             107.00         0.56136       YES     YES
    23        a             138.11         0.28842       YES     YES
    24        a             144.37         0.21805       YES     YES
    25        a             157.74         0.97101       YES     YES
    26        a             163.60         1.04911       YES     YES
    27        a             185.47         0.24484       YES     YES
    28        a             201.82         1.54103       YES     YES
    29        a             207.76         1.05400       YES     YES
    30        a             233.47         0.65986       YES     YES
    31        a             245.35         1.21255       YES     YES
    32        a             258.57         1.52062       YES     YES
    33        a             272.27         1.59868       YES     YES
    34        a             289.99         0.13259       YES     YES
    35        a             311.62         4.20087       YES     YES
    36        a             329.43         1.98900       YES     YES
    37        a             362.92         2.40152       YES     YES
    38        a             377.48         2.46814       YES     YES
    39        a             395.04        12.41401       YES     YES
    40        a             403.33         0.34388       YES     YES
    41        a             407.17         0.15896       YES     YES
    42        a             426.10         2.97114       YES     YES
    43        a             440.77         1.24828       YES     YES
    44        a             452.05         1.61406       YES     YES
    45        a             459.30         0.36019       YES     YES
    46        a             463.85         1.07994       YES     YES
    47        a             479.01         2.34965       YES     YES
    48        a             485.60         1.09251       YES     YES
    49        a             490.13         4.05355       YES     YES
    50        a             497.90         6.21632       YES     YES
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3ca'

SCF Energy (au) BP86/SV(P) -2678.218280289
SCF Energy (au) PBE0/def2-TZVPP -2677.737373921
SCF Energy (au) PBE0/def2-TZVPP -2677.7503837273 (Toluene Correction)
Zero Point Energy (au) 0.4178331
Chemical Potential (kJ mol^{-1}) 923.56
Dispersion Correction (au) PBE0/def2-TZVPP -0.08515989

xyz coordinates
57

Mn	0.2297979	2.1745138	-1.3347197
C	1.6171610	2.8337007	-0.3315315
C	1.2911652	1.0907227	-2.2971892
C	0.3343992	3.4203114	-2.5789391
O	0.3609910	4.2469473	-3.4069981
O	1.9707290	0.3987678	-2.9452103
O	2.5256098	3.2620245	0.2634741
C	-1.4768114	2.3038411	0.8307032
C	-1.8780000	4.2761384	-0.3609654
C	-2.8525899	4.6790307	0.5633144
C	-3.1316419	3.8533537	1.6646649
C	-2.4288200	2.6441698	1.8034043
C	-0.6369008	1.0678879	0.8411725
C	-0.7131995	0.1374552	-0.2162608
C	0.1030264	-1.0946837	-0.1478118
N	0.9108383	-1.2652747	1.0291886
C	0.9564707	-0.3417857	2.0553849
C	0.1983591	0.8129073	1.9730585
H	-1.6156147	4.8907832	-1.2371658
H	-3.3824773	5.6328345	0.4151367
H	-3.8916590	4.1451546	2.4072869
H	-2.6179118	1.9615775	2.6460739
O	0.1013544	-1.9604783	-1.0212301
C	1.8320981	-0.6166457	3.2481219
H	0.2658504	1.5549755	2.7813309
N	-1.2054328	3.1165711	-0.2206989
H	-1.9357513	1.5131526	-3.1078177
C	-1.3585129	1.2726871	-2.1953513
C	-1.6781994	0.2414852	-1.3724655
C	-2.7915273	-0.7316675	-1.4904575
H	1.8106211	0.2490556	3.9400695
H	2.8864511	-0.8003277	2.9471307
H	1.4896528	-1.5130903	3.8135666
C	1.6729266	-2.5335254	1.0922998
H	1.5523006	-2.9724171	2.1030852
C	3.1473011	-2.4144786	0.7377724
H	1.1659724	-3.1938085	0.3581996
C	5.8898231	-2.2723622	0.0562233
C	5.4959697	-2.8570271	1.2710702
C	4.1330585	-2.9234494	1.6086874
C	3.5518096	-1.8408847	-0.4872837
C	4.9135787	-1.7658983	-0.8204193
H	6.9582646	-2.2136907	-0.2098935
H	6.2524496	-3.2618886	1.9637387
H	3.8306678	-3.3859600	2.5648116
H	2.7967394	-1.4638642	-1.1954814
H	5.2116198	-1.3127252	-1.7801833
C	-4.9711082	-2.5509902	-1.6925383
C	-4.3148150	-2.3649062	-0.4643236
C	-3.2400184	-1.4672536	-0.3665762
C	-3.4592078	-0.9391965	-2.7228957
C	-4.5351303	-1.8314917	-2.8212454

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H    -5.8131660   -3.2582268   -1.7737531
H    -4.6427955   -2.9243449    0.4282348
H    -2.7419062   -1.3250928    0.6078718
H    -3.1110665   -0.4038709   -3.6210112
H    -5.0327927   -1.9787415   -3.7946602

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1                       0.00         0.00000        -       -
     2                       0.00         0.00000        -       -
     3                       0.00         0.00000        -       -
     4                       0.00         0.00000        -       -
     5                       0.00         0.00000        -       -
     6                       0.00         0.00000        -       -
     7        a             19.21         0.16432       YES     YES
     8        a             23.47         0.45449       YES     YES
     9        a             29.88         0.64780       YES     YES
    10        a             39.48         0.08769       YES     YES
    11        a             42.64         0.43937       YES     YES
    12        a             44.77         2.00535       YES     YES
    13        a             49.07         0.67123       YES     YES
    14        a             55.87         0.47658       YES     YES
    15        a             69.43         1.32303       YES     YES
    16        a             73.15         0.50441       YES     YES
    17        a             81.07         0.52119       YES     YES
    18        a             90.08         0.21952       YES     YES
    19        a             94.00         0.36477       YES     YES
    20        a             97.20         1.86791       YES     YES
    21        a            101.54         0.45680       YES     YES
    22        a            109.42         0.68332       YES     YES
    23        a            137.50         0.11320       YES     YES
    24        a            144.65         2.13129       YES     YES
    25        a            160.28         0.50306       YES     YES
    26        a            181.46         0.53773       YES     YES
    27        a            191.63         0.15253       YES     YES
    28        a            197.91         1.11741       YES     YES
    29        a            224.72         1.58425       YES     YES
    30        a            233.22         0.59602       YES     YES
    31        a            240.86         0.33051       YES     YES
    32        a            257.01         0.35306       YES     YES
    33        a            262.34         1.02785       YES     YES
    34        a            295.93         0.90626       YES     YES
    35        a            316.02         0.73711       YES     YES
    36        a            319.52         4.67888       YES     YES
    37        a            361.51         1.02386       YES     YES
    38        a            378.85         1.70818       YES     YES
    39        a            403.51         0.14089       YES     YES
    40        a            404.39         0.54864       YES     YES
    41        a            422.33         1.59328       YES     YES
    42        a            428.18         1.08852       YES     YES
    43        a            434.15         6.12589       YES     YES
    44        a            455.16         4.69089       YES     YES
    45        a            463.52         0.55268       YES     YES
    46        a            466.18         0.63456       YES     YES
    47        a            477.75         2.37488       YES     YES
    48        a            489.32         1.31633       YES     YES
    49        a            491.10         3.15360       YES     YES
    50        a            507.95         6.32814       YES     YES
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3da

SCF Energy (au) BP86/SV(P) -2409.037058188
SCF Energy (au) PBE0/def2-TZVPP -2408.578577113
SCF Energy (au) PBE0/def2-TZVPP -2408.5876200366 (Toluene Correction)
Zero Point Energy (au) 0.3203729
Chemical Potential (kJ mol^{-1}) 693.96
Dispersion Correction (au) PBE0/def2-TZVPP -0.06859816

xyz coordinates
45

Mn	1.1173719	1.0312839	0.3566833
C	1.5853652	1.5750691	2.0338526
C	2.7562093	0.3798074	-0.0005427
C	1.4880160	2.6264045	-0.3098843
O	1.6808120	3.7068467	-0.7146336
O	3.8142952	-0.0423134	-0.2474111
O	1.9234554	1.9382031	3.0908395
C	-1.2016639	0.0794117	1.0776690
C	-1.8119419	2.2544276	0.5093869
C	-3.1491854	1.9891519	0.8413571
C	-3.4998775	0.7133415	1.3151695
C	-2.5040187	-0.2736911	1.4376583
N	-0.0460866	-0.7976603	1.1110116
C	0.0622448	-1.7181936	-0.0254837
C	0.2544036	-2.9977070	0.4507647
C	0.3053010	-2.9554018	1.8977565
C	0.1182089	-1.6011429	2.2925356
H	-1.4764482	3.2355907	0.1375581
H	-3.9049751	2.7820805	0.7301525
H	-4.5432122	0.4829444	1.5843137
H	-2.7234604	-1.2890434	1.8000928
H	0.4354268	-3.8781585	-0.1795344
C	0.0947015	-1.1989255	3.6301130
N	-0.8640865	1.3059838	0.6397878
C	0.5895501	0.8093864	-2.7920829
C	1.7257682	1.5142081	-3.2664243
C	1.7502745	2.0697311	-4.5537556
C	0.6308816	1.9615782	-5.3988076
C	-0.5109802	1.2790708	-4.9444412
C	-0.5287534	0.7059350	-3.6634394
H	2.6131224	1.6035099	-2.6204160
H	2.6539177	2.5990724	-4.8995892
H	0.6476101	2.4121817	-6.4050893
H	-1.3988180	1.1925165	-5.5935540
H	-1.4314143	0.1808745	-3.3093448
C	0.5521816	0.1851989	-1.4555397
C	0.0988969	-1.1088118	-1.3318299
H	-0.1416297	-1.7453257	-2.2054555
C	0.2843591	-2.1930636	4.6094536
H	-0.0474494	-0.1445334	3.9121403
H	0.2843663	-1.9096302	5.6742443
C	0.4924938	-3.5405921	4.2422694
H	0.6490521	-4.2965513	5.0294823
C	0.5065170	-3.9343051	2.8944337
H	0.6691984	-4.9887601	2.6185332

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	28.92	0.40565	YES	YES
8	a	37.26	0.06249	YES	YES
9	a	46.50	0.25372	YES	YES
10	a	54.32	0.01770	YES	YES
11	a	60.74	0.30107	YES	YES
12	a	69.85	1.24702	YES	YES
13	a	74.70	0.45702	YES	YES
14	a	81.89	0.81541	YES	YES
15	a	84.73	0.24313	YES	YES
16	a	95.20	0.25017	YES	YES
17	a	98.42	0.55231	YES	YES
18	a	109.24	0.18919	YES	YES
19	a	141.07	0.11060	YES	YES
20	a	152.17	1.49613	YES	YES
21	a	180.10	1.27728	YES	YES
22	a	189.89	0.05206	YES	YES
23	a	208.92	0.97205	YES	YES
24	a	223.73	0.79529	YES	YES
25	a	261.43	0.47915	YES	YES
26	a	268.90	2.74244	YES	YES
27	a	286.18	0.52435	YES	YES
28	a	325.79	2.71826	YES	YES
29	a	363.13	0.70236	YES	YES
30	a	396.44	2.80952	YES	YES
31	a	406.95	1.05324	YES	YES
32	a	423.82	1.01802	YES	YES
33	a	435.22	11.95528	YES	YES
34	a	448.51	2.81685	YES	YES
35	a	459.52	2.65076	YES	YES
36	a	471.73	0.78697	YES	YES
37	a	481.06	0.16180	YES	YES
38	a	490.42	1.12418	YES	YES
39	a	493.26	0.25020	YES	YES
40	a	507.66	6.69919	YES	YES
41	a	517.95	6.01909	YES	YES
42	a	523.84	3.06030	YES	YES
43	a	538.84	2.98628	YES	YES
44	a	557.16	6.48803	YES	YES
45	a	576.80	1.67949	YES	YES
46	a	590.09	2.39371	YES	YES
47	a	596.12	0.77841	YES	YES
48	a	613.34	0.49274	YES	YES
49	a	615.28	7.44090	YES	YES
50	a	629.75	37.33445	YES	YES

3da'

SCF Energy (au) BP86/SV(P) -2409.034407606
SCF Energy (au) PBE0/def2-TZVPP -2408.576885875
SCF Energy (au) PBE0/def2-TZVPP -2408.5859493044 (Toluene Correction)
Zero Point Energy (au) 0.3203032
Chemical Potential (kJ mol^{-1}) 693.18
Dispersion Correction (au) PBE0/def2-TZVPP -0.06741973

xyz coordinates
45

Mn	1.4340079	1.9877711	0.3062720
C	1.8611104	2.6173755	1.9720891
C	3.0597099	1.2662607	0.0417952
C	1.8808437	3.4962167	-0.4980946
O	2.1288308	4.4943936	-1.0556917
O	4.1060042	0.7903219	-0.1480240
O	2.1753840	3.0340469	3.0164158
C	-0.9286730	1.0876959	0.9320402
C	-1.4806415	3.2806788	0.3782828
C	-2.8348031	3.0320744	0.6504191
C	-3.2248963	1.7542155	1.0856839
C	-2.2501376	0.7493288	1.2310873
N	0.2117614	0.1930013	1.0060692
C	0.3495094	-0.7519616	-0.1065452
C	0.5573961	-2.0135000	0.4037625
C	0.5762752	-1.9380122	1.8512294
C	0.3552348	-0.5798653	2.2096329
H	-1.1154830	4.2629505	0.0383258
H	-3.5728545	3.8391420	0.5229589
H	-4.2819412	1.5362782	1.3074368
H	-2.4999159	-0.2679966	1.5676158
H	0.7611768	-2.9052401	-0.2026803
C	0.2927999	-0.1486692	3.5373096
N	-0.5541226	2.3152395	0.5282990
H	1.0509728	1.6100614	-2.4509835
C	0.9377638	1.1242993	-1.4614443
C	0.4414493	-0.1591618	-1.4407637
C	0.0770928	-0.9643189	-2.6393310
C	0.4769828	-1.1177742	4.5419780
H	0.1261389	0.9089574	3.7929121
H	0.4459442	-0.8111523	5.5998927
C	0.7192618	-2.4689522	4.2107376
H	0.8712784	-3.2040692	5.0182099
C	0.7725838	-2.8913423	2.8727324
H	0.9617283	-3.9479961	2.6232848
C	-0.6553254	-2.4477331	-4.9556920
C	-1.3339412	-2.6473684	-3.7412208
C	-0.9712341	-1.9166997	-2.5986553
C	0.7560605	-0.7835335	-3.8694422
C	0.3924769	-1.5111278	-5.0121335
H	-0.9365524	-3.0241700	-5.8526284
H	-2.1586505	-3.3776792	-3.6821766
H	-1.5211851	-2.0737152	-1.6559985
H	1.5978745	-0.0739001	-3.9198092
H	0.9427041	-1.3543704	-5.9551583

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	30.85	0.31969	YES	YES
8	a	38.66	0.26769	YES	YES
9	a	44.03	0.45409	YES	YES
10	a	50.44	0.46117	YES	YES
11	a	58.79	0.13910	YES	YES
12	a	70.56	0.77444	YES	YES
13	a	73.15	0.79337	YES	YES
14	a	79.09	0.77549	YES	YES
15	a	85.25	0.31938	YES	YES
16	a	89.55	0.27598	YES	YES
17	a	96.42	0.02125	YES	YES
18	a	98.81	0.32592	YES	YES
19	a	143.17	0.26355	YES	YES
20	a	148.26	1.57227	YES	YES
21	a	186.79	0.69674	YES	YES
22	a	201.64	0.61927	YES	YES
23	a	213.25	0.94402	YES	YES
24	a	243.77	0.81043	YES	YES
25	a	254.48	0.62309	YES	YES
26	a	265.85	1.47357	YES	YES
27	a	284.54	2.00587	YES	YES
28	a	321.31	0.94779	YES	YES
29	a	355.83	1.61262	YES	YES
30	a	405.73	0.07009	YES	YES
31	a	409.56	3.84672	YES	YES
32	a	424.95	1.86710	YES	YES
33	a	428.29	0.73869	YES	YES
34	a	435.15	11.43486	YES	YES
35	a	456.30	2.74287	YES	YES
36	a	469.32	1.54325	YES	YES
37	a	479.73	0.92292	YES	YES
38	a	480.02	2.45529	YES	YES
39	a	490.24	1.33349	YES	YES
40	a	510.11	1.02306	YES	YES
41	a	517.63	12.22340	YES	YES
42	a	535.70	3.25324	YES	YES
43	a	544.60	13.91874	YES	YES
44	a	559.29	0.84540	YES	YES
45	a	586.19	12.01317	YES	YES
46	a	591.95	7.84937	YES	YES
47	a	612.80	1.80156	YES	YES
48	a	614.86	8.34012	YES	YES
49	a	623.92	17.83804	YES	YES
50	a	629.15	19.67110	YES	YES

3ea

SCF Energy (au) BP86/SV(P)	-2583.785980288
SCF Energy (au) PBE0/def2-TZVPP	-2583.339566677
SCF Energy (au) PBE0/def2-TZVPP	-2583.3503113936 (Toluene Correction)
Zero Point Energy (au)	0.3875299
Chemical Potential (kJ mol^{-1})	845.24
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07468328

xyz coordinates
53

Mn	1.9651695	1.7154598	-0.0109753
C	2.3480792	2.1006590	1.7392816
C	3.6973241	1.7465730	-0.5034005
C	1.7741513	3.3973560	-0.4504732
O	1.6051695	4.5182711	-0.7493858
O	4.8192058	1.7633187	-0.8235393
O	2.6033358	2.3533202	2.8488849
C	-0.4596660	0.2929554	0.8343070
C	-1.8865719	0.1335204	1.1967370
C	0.5060078	-0.8137106	1.0092949
C	1.4409848	-1.1567847	-0.0335687
C	2.3040319	-2.2512157	0.2004136
C	2.3034134	-2.9730490	1.4097088
C	1.3855560	-2.6246036	2.4298631
C	0.4961805	-1.5686285	2.2040837
H	3.0127941	-2.5634002	-0.5827856
O	3.2069497	-3.9838538	1.5007735
H	1.3545968	-3.1654988	3.3862966
H	-0.2292973	-1.3047793	2.9906630
N	0.0196209	1.4114102	0.3521336
C	1.4688948	1.2072974	-3.1371296
C	2.2378999	2.2996925	-3.6143953
C	2.1892361	2.6901570	-4.9601881
C	1.3497766	2.0180364	-5.8664389
C	0.5608614	0.9467961	-5.4106367
C	0.6209091	0.5470609	-4.0678958
H	2.8950311	2.8414346	-2.9166392
H	2.8091079	3.5353018	-5.3038577
H	1.3020567	2.3353389	-6.9215125
H	-0.1133541	0.4207023	-6.1077445
H	-0.0163634	-0.2805926	-3.7138587
C	1.5237799	0.7697178	-1.7339513
C	1.4568059	-0.5578925	-1.3974224
H	1.5804506	-1.3178251	-2.1995321
C	-4.6486942	-0.1440778	1.8216597
C	-3.8957116	-1.2585711	1.3794449
C	-2.5409938	-1.1210499	1.0794103
C	-2.6500765	1.2351825	1.6485544
C	-4.0110524	1.1102307	1.9590232
O	-5.9571818	-0.3790843	2.0947564
H	-4.4092359	-2.2272115	1.2753295
H	-1.9733789	-1.9956395	0.7236929
H	-2.1637524	2.2140225	1.7981964
H	-4.5601925	1.9905313	2.3235603
H	-0.6890552	2.1269921	0.1307717
C	-6.7749949	0.6979217	2.5289010
H	-6.4171042	1.1218142	3.4963019
H	-7.7888033	0.2737619	2.6716324
H	-6.8227436	1.5107816	1.7666559
C	3.2675396	-4.7477234	2.6950863
H	2.3081708	-5.2818123	2.8928381
H	3.5230979	-4.1143063	3.5769682

H 4.0720346 -5.4943078 2.5401061

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.51	0.31178	YES	YES
8	a	20.08	0.83075	YES	YES
9	a	25.76	0.14120	YES	YES
10	a	37.40	0.41839	YES	YES
11	a	41.74	0.36272	YES	YES
12	a	49.73	0.66072	YES	YES
13	a	55.73	0.02701	YES	YES
14	a	59.24	0.47353	YES	YES
15	a	72.72	1.11749	YES	YES
16	a	82.52	2.52930	YES	YES
17	a	85.90	0.32333	YES	YES
18	a	88.22	0.71131	YES	YES
19	a	96.11	0.90403	YES	YES
20	a	103.97	1.16949	YES	YES
21	a	114.15	0.83859	YES	YES
22	a	128.32	0.20179	YES	YES
23	a	146.83	0.31438	YES	YES
24	a	151.89	1.29281	YES	YES
25	a	168.11	4.09408	YES	YES
26	a	179.42	1.14541	YES	YES
27	a	200.02	0.38012	YES	YES
28	a	207.62	1.66963	YES	YES
29	a	226.15	1.86463	YES	YES
30	a	235.19	0.92040	YES	YES
31	a	239.41	4.04946	YES	YES
32	a	255.06	2.65217	YES	YES
33	a	269.98	4.48469	YES	YES
34	a	295.05	0.80520	YES	YES
35	a	302.33	8.55660	YES	YES
36	a	321.72	4.90520	YES	YES
37	a	332.49	0.29942	YES	YES
38	a	369.86	2.17629	YES	YES
39	a	406.94	0.53710	YES	YES
40	a	414.79	0.71808	YES	YES
41	a	423.67	13.01661	YES	YES
42	a	438.34	2.17459	YES	YES
43	a	443.47	3.37086	YES	YES
44	a	459.10	0.73837	YES	YES
45	a	466.53	1.15636	YES	YES
46	a	479.54	5.36961	YES	YES
47	a	486.06	4.36720	YES	YES
48	a	487.99	0.66771	YES	YES
49	a	508.96	4.99059	YES	YES
50	a	517.77	16.82526	YES	YES

3ea'

SCF Energy (au) BP86/SV(P)	-2583.783208244
SCF Energy (au) PBE0/def2-TZVPP	-2583.338085995
SCF Energy (au) PBE0/def2-TZVPP	-2583.3490964570 (Toluene Correction)
Zero Point Energy (au)	0.3874885
Chemical Potential (kJ mol^{-1})	845.08
Dispersion Correction (au) PBE0/def2-TZVPP	-0.07655516

xyz coordinates
53

Mn	2.2974223	2.1044248	0.4369364
C	2.5307348	2.4894570	2.2189721
C	3.9961773	1.5489878	0.2111146
C	2.6950408	3.7214756	-0.1135425
O	2.9172068	4.8004252	-0.5113261
O	5.0878474	1.1750973	0.0386081
O	2.7266135	2.7509417	3.3388771
C	-0.3367679	1.2586260	0.8293903
C	0.5650690	0.0931635	1.0974360
C	1.4190804	-0.4432591	0.0796196
C	2.2302767	-1.5631004	0.3996120
C	2.2196428	-2.1378792	1.6817671
C	1.3580732	-1.6084829	2.6786297
C	0.5452219	-0.5219353	2.3808379
H	2.8695718	-1.9689312	-0.3975123
O	2.9841743	-3.1913069	2.0626043
H	1.3581999	-2.0726174	3.6768799
H	-0.1263325	-0.1178035	3.1557622
N	0.3099283	2.3397319	0.4920302
H	2.0412466	1.8893515	-2.3888246
C	1.9315377	1.3882431	-1.4079445
C	1.4722862	0.1082100	-1.3263266
C	1.0943724	-0.7792518	-2.4587611
C	0.3152161	-2.4467361	-4.6381530
C	-0.1268456	-2.7283626	-3.3346308
C	0.2589812	-1.9081774	-2.2623096
C	1.5376021	-0.5183121	-3.7808919
C	1.1510932	-1.3346910	-4.8523306
H	0.0166338	-3.0916677	-5.4811835
H	-0.7832348	-3.5953591	-3.1483465
H	-0.1036392	-2.1414395	-1.2473626
H	2.2121393	0.3334013	-3.9649028
H	1.5166260	-1.1071508	-5.8679953
H	-0.2535891	3.1571260	0.2143462
C	-1.8001614	1.1572467	0.9782788
C	-4.6305559	0.9519304	1.2004177
C	-3.9975071	2.2132014	1.3019330
C	-2.6042064	2.3022971	1.1927338
C	-2.4532462	-0.1014638	0.8965114
C	-3.8394319	-0.2047556	0.9993735
O	-5.9688860	0.7507156	1.2899569
H	-4.5802896	3.1284535	1.4809860
H	-2.1331432	3.2929831	1.3085166
H	-1.8544808	-1.0106545	0.7282756
H	-4.3478546	-1.1784593	0.9226608
C	-6.8248518	1.8678565	1.4820771
H	-7.8555108	1.4617076	1.5106249
H	-6.7418905	2.5971653	0.6426280
H	-6.6108553	2.3890134	2.4446946
C	3.8940188	-3.7532632	1.1255572
H	4.6405768	-3.0004128	0.7809828
H	3.3628970	-4.1761989	0.2411378

H 4.4177724 -4.5695610 1.6615739

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.63	0.19309	YES	YES
8	a	21.60	0.77485	YES	YES
9	a	27.86	0.18949	YES	YES
10	a	35.39	0.38876	YES	YES
11	a	41.33	0.19663	YES	YES
12	a	44.02	0.29313	YES	YES
13	a	46.80	0.16734	YES	YES
14	a	56.38	0.54129	YES	YES
15	a	66.90	0.05337	YES	YES
16	a	79.52	0.12712	YES	YES
17	a	82.08	0.21891	YES	YES
18	a	91.71	0.53619	YES	YES
19	a	94.79	0.47801	YES	YES
20	a	104.40	2.24284	YES	YES
21	a	118.46	1.63451	YES	YES
22	a	134.87	1.59926	YES	YES
23	a	146.93	1.29975	YES	YES
24	a	160.54	2.27608	YES	YES
25	a	164.22	0.42093	YES	YES
26	a	178.65	1.05013	YES	YES
27	a	184.01	0.32613	YES	YES
28	a	208.70	2.55452	YES	YES
29	a	212.55	0.03873	YES	YES
30	a	239.72	0.04436	YES	YES
31	a	260.67	0.38034	YES	YES
32	a	270.38	1.24015	YES	YES
33	a	272.85	4.07023	YES	YES
34	a	298.06	9.95050	YES	YES
35	a	313.32	0.41120	YES	YES
36	a	318.07	1.89895	YES	YES
37	a	342.89	2.41294	YES	YES
38	a	403.82	0.05490	YES	YES
39	a	411.48	0.65777	YES	YES
40	a	417.18	2.58456	YES	YES
41	a	423.43	8.11935	YES	YES
42	a	439.84	3.47479	YES	YES
43	a	453.26	0.80939	YES	YES
44	a	454.51	2.07382	YES	YES
45	a	462.67	2.46979	YES	YES
46	a	473.90	0.79383	YES	YES
47	a	486.97	4.80856	YES	YES
48	a	491.01	1.88003	YES	YES
49	a	508.87	18.13092	YES	YES
50	a	515.17	21.25998	YES	YES

3ej

SCF Energy (au) BP86/SV(P)	-2814.675728998
SCF Energy (au) PBE0/def2-TZVPP	-2814.194226758
SCF Energy (au) PBE0/def2-TZVPP	-2814.2067699821
Zero Point Energy (au)	0.4661736
Chemical Potential (kJ mol^{-1})	1036.22
Dispersion Correction (au) PBE0/def2-TZVPP	-0.09605401

xyz coordinates

63

Mn	1.8614852	1.8272271	0.7600694
C	2.1430144	2.1835792	2.5350904
C	3.6016826	1.4888872	0.4378122
C	2.0500388	3.5079382	0.2825505
O	2.1338044	4.6332195	-0.0284058
O	4.7256063	1.2775391	0.2046422
O	2.3623552	2.4227320	3.6562518
C	-0.6663726	0.7692076	1.3127486
C	-2.1059430	0.5460214	1.5349114
C	0.3567525	-0.2822895	1.5951215
C	1.2683272	-0.7312598	0.5727640
C	2.2161006	-1.7194815	0.9236190
C	2.3031394	-2.2513658	2.2233758
C	1.3933620	-1.8126449	3.2182310
C	0.4345636	-0.8518925	2.8895608
H	2.9102648	-2.1009480	0.1590779
O	3.2741955	-3.1777885	2.4271941
H	1.4299679	-2.2109247	4.2423712
H	-0.2749580	-0.5153012	3.6629406
N	-0.1318268	1.8801622	0.8840006
C	1.3685189	1.7584076	-2.3716643
C	2.4382710	2.5544955	-2.8558632
C	2.3323582	3.2495815	-4.0700113
C	1.1444819	3.1943154	-4.8210521
C	0.0650148	2.4276527	-4.3461588
C	0.1764819	1.7142486	-3.1433719
H	3.3698502	2.6152232	-2.2702919
H	3.1851013	3.8506290	-4.4281487
H	1.0581312	3.7523870	-5.7681421
H	-0.8747790	2.3805308	-4.9221699
H	-0.6704910	1.1094425	-2.7804303
C	1.4573975	1.0464670	-1.0879726
C	1.1980761	-0.2803654	-0.8690963
C	0.9720158	-1.3465352	-1.8889216
C	-4.8941321	0.1039928	1.9039173
C	-4.0078525	-0.9885286	1.7460380
C	-2.6427381	-0.7687003	1.5695352
C	-3.0037724	1.6266523	1.7078248
C	-4.3771537	1.4209155	1.8878551
O	-6.2033108	-0.2092240	2.0707061
H	-4.4261663	-2.0069376	1.7604853
H	-1.9693135	-1.6301234	1.4357209
H	-2.6227897	2.6613351	1.7321583
H	-5.0348254	2.2906856	2.0302847
H	-0.7729605	2.6285282	0.5818223
C	-7.1518246	0.8383416	2.2158342
H	-6.9520461	1.4508053	3.1261551
H	-8.1385144	0.3447221	2.3199327
H	-7.1681416	1.5035833	1.3209379
C	3.4333409	-3.7393500	3.7213342
H	2.5244138	-4.3010910	4.0423651
H	3.6718864	-2.9596801	4.4819780

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H     4.2852339   -4.4442321    3.6450391
C     0.5273194   -3.4043260   -3.8078954
C    -0.1128372   -3.4508009   -2.5573833
C     0.1115124   -2.4386197   -1.6112747
C     1.6196019   -1.3247218   -3.1499652
C     1.3975103   -2.3370985   -4.0950872
H     0.3562515   -4.2003302   -4.5515579
H    -0.7944227   -4.2836290   -2.3148456
H    -0.3988472   -2.4876558   -0.6346783
H     2.3189617   -0.5071702   -3.3820013
H     1.9196277   -2.2964399   -5.0658676

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)      km/mol          IR     RAMAN
     1                       0.00        0.00000        -       -
     2                       0.00        0.00000        -       -
     3                       0.00        0.00000        -       -
     4                       0.00        0.00000        -       -
     5                       0.00        0.00000        -       -
     6                       0.00        0.00000        -       -
     7        a             16.39        0.11460       YES     YES
     8        a             21.37        0.06926       YES     YES
     9        a             27.70        0.35408       YES     YES
    10        a             34.81        0.58605       YES     YES
    11        a             36.88        0.42762       YES     YES
    12        a             45.70        0.11059       YES     YES
    13        a             47.61        0.39275       YES     YES
    14        a             50.03        0.43572       YES     YES
    15        a             54.24        0.47325       YES     YES
    16        a             56.72        0.23312       YES     YES
    17        a             66.85        0.24090       YES     YES
    18        a             73.98        0.70798       YES     YES
    19        a             83.56        0.35825       YES     YES
    20        a             86.20        0.95309       YES     YES
    21        a             89.67        0.50301       YES     YES
    22        a             98.55        0.80454       YES     YES
    23        a            103.82        1.38037       YES     YES
    24        a            117.97        0.55286       YES     YES
    25        a            130.79        1.31610       YES     YES
    26        a            146.21        0.78006       YES     YES
    27        a            149.50        0.24248       YES     YES
    28        a            154.90        1.76928       YES     YES
    29        a            174.48        1.03601       YES     YES
    30        a            188.27        0.72738       YES     YES
    31        a            204.30        1.41449       YES     YES
    32        a            216.12        0.28070       YES     YES
    33        a            229.06        0.17449       YES     YES
    34        a            232.97        1.30367       YES     YES
    35        a            241.26        1.73607       YES     YES
    36        a            250.95        1.60374       YES     YES
    37        a            253.42        1.45897       YES     YES
    38        a            260.82        1.45105       YES     YES
    39        a            295.61        3.47743       YES     YES
    40        a            296.85        2.88335       YES     YES
    41        a            319.22        3.17226       YES     YES
    42        a            346.77        0.76517       YES     YES
    43        a            401.35        0.73305       YES     YES
    44        a            403.69        0.30821       YES     YES
    45        a            406.71        0.54868       YES     YES
    46        a            413.00        0.48532       YES     YES
    47        a            432.96        2.64496       YES     YES
    48        a            436.95       11.61757       YES     YES
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49	a	445.85	6.05936	YES	YES
50	a	458.16	3.03188	YES	YES

3fa

SCF Energy (au) BP86/SV(P) -2391.992336901
SCF Energy (au) PBE0/def2-TZVPP -2391.554013615
SCF Energy (au) PBE0/def2-TZVPP -2391.5628786450 (Toluene Correction)
Zero Point Energy (au) 0.3230498
Chemical Potential (kJ mol^{-1}) 696.59
Dispersion Correction (au) PBE0/def2-TZVPP -0.06995959

xyz coordinates
45

Mn	1.3893256	0.0876337	0.7929616
C	1.9375193	0.2572834	2.5295937
C	2.9494388	-0.6115109	0.2520024
C	1.9693035	1.6982189	0.3876714
O	2.3914858	2.7574452	0.1236272
O	3.9613387	-1.0608219	-0.1172982
O	2.3248523	0.3716485	3.6248438
C	-1.1604195	-0.6563062	1.6342081
C	-1.2997661	1.6357765	1.1543460
C	-2.6639989	1.6633687	1.5209604
C	-3.2631552	0.4780593	1.9666187
C	-2.5078469	-0.7036217	2.0277464
C	-0.2731292	-1.8579394	1.6496923
C	0.2795776	-2.3939772	0.4371837
C	0.9424123	-3.6500144	0.5190256
C	1.0927035	-4.3297003	1.7297636
C	0.5719453	-3.7794209	2.9200566
C	-0.1155225	-2.5648225	2.8710743
O	-0.5978210	2.6959424	0.7265859
H	-3.2432555	2.5949506	1.4605104
H	-4.3259905	0.4779088	2.2582762
H	-2.9490841	-1.6574740	2.3522989
H	1.3483386	-4.0826774	-0.4104427
H	1.6229371	-5.2962157	1.7540469
H	0.6957706	-4.3060604	3.8800926
H	-0.5497869	-2.1386511	3.7905931
N	-0.5745361	0.4961078	1.2257988
C	0.5399501	0.2680166	-2.3132376
C	1.6306738	1.0208220	-2.8181526
C	1.5528546	1.6673793	-4.0605371
C	0.3748659	1.6006528	-4.8265155
C	-0.7237283	0.8716036	-4.3376641
C	-0.6410425	0.2119474	-3.1015705
H	2.5602130	1.0809591	-2.2308591
H	2.4224991	2.2343528	-4.4334197
H	0.3123101	2.1192231	-5.7977797
H	-1.6560547	0.8162619	-4.9252319
H	-1.5090957	-0.3495544	-2.7178697
C	0.6145950	-0.4458345	-1.0281940
C	0.1482964	-1.7181938	-0.8798387
H	-0.1964605	-2.3395073	-1.7343853
C	-1.2373787	3.9568516	0.5722660
H	-2.0652377	3.9017843	-0.1713883
H	-0.4521083	4.6418740	0.1979794
H	-1.6277885	4.3362318	1.5445606

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	28.02	0.61831	YES	YES
8	a	35.88	0.12888	YES	YES
9	a	40.30	0.55568	YES	YES
10	a	46.39	0.18241	YES	YES
11	a	54.16	0.21157	YES	YES
12	a	59.73	0.20736	YES	YES
13	a	71.76	1.45852	YES	YES
14	a	79.33	0.73701	YES	YES
15	a	86.90	0.34167	YES	YES
16	a	95.76	0.47929	YES	YES
17	a	102.86	0.18488	YES	YES
18	a	115.16	0.56838	YES	YES
19	a	116.40	1.09103	YES	YES
20	a	136.46	0.21938	YES	YES
21	a	145.56	1.21576	YES	YES
22	a	170.97	0.23423	YES	YES
23	a	183.55	0.65378	YES	YES
24	a	191.89	0.07650	YES	YES
25	a	207.95	0.58322	YES	YES
26	a	236.01	0.87400	YES	YES
27	a	261.57	0.19107	YES	YES
28	a	268.32	0.04572	YES	YES
29	a	293.06	1.07449	YES	YES
30	a	314.39	0.85664	YES	YES
31	a	326.70	1.24900	YES	YES
32	a	359.74	1.05307	YES	YES
33	a	407.02	0.18747	YES	YES
34	a	411.91	1.53031	YES	YES
35	a	443.70	2.15286	YES	YES
36	a	454.02	2.16238	YES	YES
37	a	464.43	3.10826	YES	YES
38	a	470.00	2.56835	YES	YES
39	a	475.86	2.54220	YES	YES
40	a	482.34	5.04952	YES	YES
41	a	498.98	1.16430	YES	YES
42	a	517.77	5.41991	YES	YES
43	a	526.65	3.00938	YES	YES
44	a	538.96	3.75754	YES	YES
45	a	546.71	2.40756	YES	YES
46	a	552.90	6.08976	YES	YES
47	a	562.03	1.58074	YES	YES
48	a	587.33	1.67984	YES	YES
49	a	613.53	0.81749	YES	YES
50	a	621.75	26.77573	YES	YES

3fa'

SCF Energy (au) BP86/SV(P) -2391.990036695
SCF Energy (au) PBE0/def2-TZVPP -2391.552440556
SCF Energy (au) PBE0/def2-TZVPP -2391.5618337702 (Toluene Correction)
Zero Point Energy (au) 0.3230933
Chemical Potential (kJ mol^{-1}) 696.35
Dispersion Correction (au) PBE0/def2-TZVPP -0.06902345

xyz coordinates
45

Mn	1.5958874	1.2194711	0.8192433
C	1.9119078	1.6502330	2.5727878
C	3.2396413	0.5500429	0.5694944
C	2.1294424	2.7816886	0.2114912
O	2.5047679	3.7997952	-0.2258318
O	4.3043764	0.1080234	0.3896308
O	2.1565181	1.9463207	3.6751769
C	-0.9726965	0.3512824	1.3474514
C	-1.2238104	2.6135044	0.7817135
C	-2.6236647	2.5349199	0.9615354
C	-3.1820694	1.3119655	1.3556269
C	-2.3514676	0.1968958	1.5560837
C	0.0240809	-0.7483572	1.5464177
C	0.7453824	-1.3160323	0.4449884
C	1.5727749	-2.4420447	0.7078335
C	1.7033937	-2.9750288	1.9919739
C	0.9959331	-2.4048745	3.0721509
C	0.1598273	-1.3105294	2.8454942
O	-0.5535451	3.7193529	0.4183955
H	-3.2624194	3.4138406	0.7985656
H	-4.2714651	1.2304532	1.5015322
H	-2.7555639	-0.7817643	1.8540149
H	2.1196722	-2.8922407	-0.1363837
H	2.3642676	-3.8411970	2.1611832
H	1.0999333	-2.8189897	4.0880986
H	-0.4065927	-0.8644197	3.6795261
N	-0.4311686	1.5383193	0.9824148
H	1.1435329	1.0777133	-1.9829699
C	1.1108779	0.5381239	-1.0164736
C	0.6659029	-0.7479829	-0.9481779
C	0.1936539	-1.6064361	-2.0644108
C	-0.7616451	-3.2272995	-4.2059009
C	-1.0822533	-3.5470289	-2.8759322
C	-0.6110365	-2.7482870	-1.8214930
C	0.5126253	-1.3050842	-3.4133187
C	0.0393637	-2.0992962	-4.4663745
H	-1.1272918	-3.8553737	-5.0351199
H	-1.7094212	-4.4272095	-2.6544714
H	-0.8813878	-3.0085416	-0.7844734
H	1.1592413	-0.4402662	-3.6334657
H	0.3090477	-1.8425405	-5.5048191
C	-1.2657020	4.9239144	0.1631691
H	-1.9903366	4.7973859	-0.6740308
H	-0.4972931	5.6669884	-0.1255121
H	-1.8012214	5.2805898	1.0731657

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	26.43	0.64410	YES	YES
8	a	36.00	0.10988	YES	YES
9	a	39.31	0.64830	YES	YES
10	a	46.99	0.07932	YES	YES
11	a	53.88	0.60268	YES	YES
12	a	57.99	0.14448	YES	YES
13	a	78.15	0.85951	YES	YES
14	a	79.22	0.86036	YES	YES
15	a	86.49	0.36867	YES	YES
16	a	92.13	1.75821	YES	YES
17	a	96.91	0.41554	YES	YES
18	a	109.81	0.52623	YES	YES
19	a	112.58	0.93413	YES	YES
20	a	134.50	0.80920	YES	YES
21	a	151.79	0.07598	YES	YES
22	a	172.87	0.86313	YES	YES
23	a	194.28	0.18231	YES	YES
24	a	198.29	0.16023	YES	YES
25	a	218.11	0.73152	YES	YES
26	a	241.18	0.24161	YES	YES
27	a	259.58	0.18536	YES	YES
28	a	270.76	0.41493	YES	YES
29	a	285.93	0.46475	YES	YES
30	a	300.73	1.69595	YES	YES
31	a	330.64	1.18946	YES	YES
32	a	371.83	0.29010	YES	YES
33	a	404.19	0.17024	YES	YES
34	a	414.83	2.07391	YES	YES
35	a	442.03	3.05176	YES	YES
36	a	458.75	0.49513	YES	YES
37	a	466.64	2.23317	YES	YES
38	a	471.52	1.38698	YES	YES
39	a	473.56	6.02926	YES	YES
40	a	477.32	1.32248	YES	YES
41	a	495.82	2.27249	YES	YES
42	a	524.09	10.32641	YES	YES
43	a	527.91	4.64607	YES	YES
44	a	544.34	4.44421	YES	YES
45	a	551.51	6.18662	YES	YES
46	a	572.66	6.36547	YES	YES
47	a	585.87	2.13074	YES	YES
48	a	605.12	10.06900	YES	YES
49	a	612.62	11.75680	YES	YES
50	a	616.40	14.82095	YES	YES

3ga

SCF Energy (au) BP86/SV(P) -2508.432275552
SCF Energy (au) PBE0/def2-TZVPP -2507.958331998
SCF Energy (au) PBE0/def2-TZVPP -2507.9668305178 (Toluene Correction)
Zero Point Energy (au) 0.3699565
Chemical Potential (kJ mol^{-1}) 811.35
Dispersion Correction (au) PBE0/def2-TZVPP -0.08488781

xyz coordinates
51

Mn	1.2727708	-0.4332971	0.8077556
C	1.7707572	-0.1092857	2.5352243
C	2.7991138	-1.2895947	0.4156375
C	2.0107523	1.0823652	0.2975907
O	2.5731236	2.0592395	-0.0167825
O	3.7865517	-1.8502685	0.1476760
O	2.1262832	0.1019435	3.6266265
C	-1.2039849	-1.1041463	1.6676312
C	-1.4649532	1.1863673	1.1855316
C	-2.7829765	1.1473506	1.6963750
C	-3.3128516	-0.0465461	2.1956206
C	-2.5085134	-1.1959060	2.1787170
C	-0.2816629	-2.2851359	1.7060502
C	0.1710193	-2.9476128	0.5144462
C	0.7821341	-4.2238243	0.6584667
C	0.9927149	-4.8035228	1.9103597
C	0.5902302	-4.1259705	3.0824595
C	-0.0546454	-2.8940219	2.9733010
C	-0.9384016	2.4744860	0.6543132
H	-3.3838601	2.0688894	1.6725252
H	-4.3432384	-0.0855125	2.5848200
H	-2.8746612	-2.1647186	2.5513275
H	1.1086373	-4.7475062	-0.2551866
H	1.4833475	-5.7883762	1.9831589
H	0.7690507	-4.5707846	4.0745333
H	-0.4056870	-2.3746036	3.8804688
N	-0.6960826	0.0637399	1.1885210
C	0.5422277	-0.4556476	-2.3450926
C	1.6806026	0.2122683	-2.8646464
C	1.6670712	0.7770619	-4.1489600
C	0.5086847	0.7121400	-4.9447528
C	-0.6353203	0.0661173	-4.4435357
C	-0.6175203	-0.5130755	-3.1649267
H	2.5954765	0.2701861	-2.2546878
H	2.5725715	1.2772438	-4.5319369
H	0.4969203	1.1670741	-5.9491877
H	-1.5526615	0.0133452	-5.0541335
H	-1.5208462	-1.0092120	-2.7729391
C	0.5483680	-1.0846884	-1.0123511
C	0.0500190	-2.3411793	-0.8280562
H	-0.2844929	-2.9933694	-1.6624084
C	-0.1022246	4.9745170	-0.3583789
C	-0.5250942	4.8634252	0.9777925
C	-0.9495964	3.6232699	1.4789414
C	-0.5122545	2.5952404	-0.6859912
C	-0.0998301	3.8397572	-1.1866599
H	0.2288094	5.9491154	-0.7537595
H	-0.5213643	5.7475064	1.6364710
H	-1.2756174	3.5363344	2.5289025
H	-0.5093230	1.7116159	-1.3418794
H	0.2304268	3.9172061	-2.2349916

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	25.84	0.04845	YES	YES
8	a	26.55	0.02052	YES	YES
9	a	35.80	0.32049	YES	YES
10	a	39.25	0.03499	YES	YES
11	a	50.44	0.01163	YES	YES
12	a	54.68	0.65930	YES	YES
13	a	62.61	0.01939	YES	YES
14	a	69.07	0.26530	YES	YES
15	a	80.18	1.09165	YES	YES
16	a	83.57	0.18719	YES	YES
17	a	91.28	0.07543	YES	YES
18	a	106.38	0.19122	YES	YES
19	a	107.60	0.29624	YES	YES
20	a	110.51	0.06144	YES	YES
21	a	125.01	1.02495	YES	YES
22	a	143.88	0.26257	YES	YES
23	a	154.72	0.83859	YES	YES
24	a	173.13	1.39150	YES	YES
25	a	190.08	0.40542	YES	YES
26	a	198.81	0.17350	YES	YES
27	a	230.09	0.74020	YES	YES
28	a	258.49	0.10339	YES	YES
29	a	265.26	0.79766	YES	YES
30	a	299.31	0.13424	YES	YES
31	a	320.51	1.06814	YES	YES
32	a	345.08	1.58179	YES	YES
33	a	372.24	0.09462	YES	YES
34	a	379.45	1.38213	YES	YES
35	a	400.84	0.39030	YES	YES
36	a	406.61	0.47180	YES	YES
37	a	418.10	1.20687	YES	YES
38	a	448.19	0.52402	YES	YES
39	a	455.32	0.83848	YES	YES
40	a	466.65	0.88780	YES	YES
41	a	474.11	0.33446	YES	YES
42	a	489.02	4.93957	YES	YES
43	a	501.61	1.47829	YES	YES
44	a	503.21	11.56780	YES	YES
45	a	523.20	2.12663	YES	YES
46	a	532.27	2.99148	YES	YES
47	a	540.69	5.81623	YES	YES
48	a	546.42	3.39454	YES	YES
49	a	556.83	2.45245	YES	YES
50	a	559.84	2.16353	YES	YES

3ga'

SCF Energy (au) BP86/SV(P) -2508.431196130
SCF Energy (au) PBE0/def2-TZVPP -2507.957419935
SCF Energy (au) PBE0/def2-TZVPP -2507.9666554808 (Toluene Correction)
Zero Point Energy (au) 0.3699454
Chemical Potential (kJ mol^{-1}) 810.86
Dispersion Correction (au) PBE0/def2-TZVPP -0.08233166

xyz coordinates
51

Mn	1.5028971	0.4619076	0.8244350
C	1.8610594	0.9959175	2.5377272
C	3.0723701	-0.3902685	0.6581873
C	2.2134124	1.8824475	0.0628351
O	2.7210324	2.7732632	-0.4990363
O	4.0913041	-0.9452745	0.5388870
O	2.1319073	1.3619097	3.6139335
C	-1.0799484	-0.2214387	1.2500738
C	-1.2802869	2.0496447	0.6658923
C	-2.6890924	1.9284459	0.6707401
C	-3.2912878	0.7052950	0.9841893
C	-2.4703122	-0.3910427	1.2953473
C	-0.1231398	-1.3378904	1.5565186
C	0.5226403	-2.0672512	0.5052292
C	1.2369224	-3.2447021	0.8533463
C	1.3388621	-3.6695889	2.1800907
C	0.7224657	-2.9332044	3.2154580
C	-0.0086079	-1.7861231	2.9021516
C	-0.6547343	3.3735215	0.4000120
H	-3.2976659	2.8196640	0.4539523
H	-4.3890445	0.6080301	0.9977374
H	-2.8893230	-1.3749234	1.5560449
H	1.7260810	-3.8169703	0.0487384
H	1.9121756	-4.5804815	2.4201307
H	0.8104040	-3.2633623	4.2631026
H	-0.5171513	-1.2181188	3.6987699
N	-0.5033870	0.9675818	0.9360635
H	1.0805268	0.2185027	-1.9755761
C	0.9985047	-0.2854715	-0.9926964
C	0.5072780	-1.5551744	-0.9051413
C	0.0395398	-2.4266975	-2.0123330
C	-0.9095803	-4.0676480	-4.1396019
C	-1.3142116	-4.3163081	-2.8172489
C	-0.8461257	-3.5069520	-1.7695609
C	0.4428470	-2.1974358	-3.3524435
C	-0.0275756	-3.0017621	-4.3993144
H	-1.2735282	-4.7034473	-4.9636520
H	-2.0055557	-5.1473674	-2.5972797
H	-1.1830726	-3.7081036	-0.7387922
H	1.1530767	-1.3830656	-3.5690219
H	0.3076621	-2.8027175	-5.4312424
C	0.4275050	5.9411982	-0.0593172
C	0.7627062	5.2324467	1.1068621
C	0.2286643	3.9558823	1.3363159
C	-0.9986846	4.0989691	-0.7624859
C	-0.4540578	5.3716305	-0.9938517
H	0.8562097	6.9404445	-0.2417441
H	1.4492572	5.6761343	1.8462932
H	0.4867038	3.4108470	2.2577910
H	-1.6816539	3.6493267	-1.5025631
H	-0.7159876	5.9197807	-1.9139531

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	21.80	0.16220	YES	YES
8	a	28.64	0.04894	YES	YES
9	a	36.93	0.20170	YES	YES
10	a	41.81	0.24131	YES	YES
11	a	46.48	0.08780	YES	YES
12	a	56.43	0.06689	YES	YES
13	a	63.55	0.47475	YES	YES
14	a	69.71	0.08274	YES	YES
15	a	80.44	0.85743	YES	YES
16	a	83.10	0.29376	YES	YES
17	a	90.96	0.67737	YES	YES
18	a	97.65	0.51042	YES	YES
19	a	104.49	0.67564	YES	YES
20	a	109.49	0.09221	YES	YES
21	a	121.43	0.40199	YES	YES
22	a	144.90	1.16747	YES	YES
23	a	160.09	0.03778	YES	YES
24	a	175.91	0.87185	YES	YES
25	a	202.30	0.09861	YES	YES
26	a	209.00	1.87276	YES	YES
27	a	232.32	0.56181	YES	YES
28	a	247.26	0.89539	YES	YES
29	a	279.58	0.06946	YES	YES
30	a	291.77	0.24440	YES	YES
31	a	317.63	0.51329	YES	YES
32	a	332.98	1.35842	YES	YES
33	a	354.30	0.79297	YES	YES
34	a	401.06	0.13085	YES	YES
35	a	402.72	1.42056	YES	YES
36	a	404.75	0.25181	YES	YES
37	a	414.04	1.99353	YES	YES
38	a	456.26	2.32840	YES	YES
39	a	458.63	0.40697	YES	YES
40	a	466.41	1.26669	YES	YES
41	a	473.63	2.91763	YES	YES
42	a	475.99	0.58484	YES	YES
43	a	495.71	3.10966	YES	YES
44	a	507.57	5.64543	YES	YES
45	a	522.33	11.32701	YES	YES
46	a	530.23	5.55672	YES	YES
47	a	542.98	9.38660	YES	YES
48	a	555.30	2.52328	YES	YES
49	a	573.57	6.35314	YES	YES
50	a	604.68	6.94203	YES	YES

3ha

SCF Energy (au) BP86/SV(P) -2354.896525758
SCF Energy (au) PBE0/def2-TZVPP -2354.447582458
SCF Energy (au) PBE0/def2-TZVPP -2354.4561647301 (Toluene Correction)
Zero Point Energy (au) 0.3247184
Chemical Potential (kJ mol^{-1}) 698.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.06734630

45

Mn	1.8497483	1.1028289	0.4584999
C	2.3962619	1.3587991	2.1905971
C	3.5333785	0.9238504	-0.1600726
C	1.8660182	2.8121141	0.0884741
O	1.8382320	3.9560846	-0.1641401
O	4.6199855	0.8059896	-0.5663851
O	2.7520255	1.5276083	3.2875670
C	-0.7054563	-0.0098118	1.3823506
C	-2.1394295	0.0003492	1.7665265
C	0.1106602	-1.2432892	1.4872944
C	0.9370762	-1.6614085	0.3886899
C	1.6651054	-2.8726502	0.5552985
C	1.6208297	-3.6127409	1.7405413
C	0.8141070	-3.1833551	2.8134205
C	0.0544973	-2.0172268	2.6716259
H	2.2822125	-3.2274646	-0.2869896
H	2.2163630	-4.5362864	1.8305783
H	0.7747562	-3.7599084	3.7515646
H	-0.5937026	-1.6787484	3.4963007
N	-0.0911736	1.0514123	0.9302620
C	1.0975114	0.7866837	-2.6460164
C	1.9569420	1.8049844	-3.1326176
C	1.8791743	2.2488333	-4.4603469
C	0.9228710	1.7061809	-5.3368813
C	0.0454810	0.7109950	-4.8701619
C	0.1322518	0.2579281	-3.5462639
H	2.7068543	2.2457189	-2.4577649
H	2.5690828	3.0340286	-4.8122970
H	0.8536291	2.0660586	-6.3769160
H	-0.7189774	0.2877369	-5.5436486
H	-0.5735378	-0.5073957	-3.1825160
C	1.1784931	0.2943742	-1.2632088
C	0.9589983	-1.0244135	-0.9561433
H	0.9396469	-1.7668659	-1.7838619
C	-4.8945020	0.0414844	2.4180097
C	-4.3029510	-1.1350330	1.9253431
C	-2.9367949	-1.1594302	1.6077318
C	-2.7462638	1.1766638	2.2726661
C	-4.1106720	1.1961662	2.5941723
H	-5.9670312	0.0575576	2.6722177
H	-4.9124069	-2.0426069	1.7835704
H	-2.4797178	-2.0799137	1.2112054
H	-2.1355333	2.0780554	2.4498845
H	-4.5635049	2.1166377	2.9976601
H	-0.7005380	1.8694253	0.7741796

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.81	0.42118	YES	YES
8	a	25.24	0.76632	YES	YES
9	a	32.01	0.00412	YES	YES
10	a	48.45	0.03318	YES	YES
11	a	51.30	0.16810	YES	YES
12	a	54.97	0.07239	YES	YES
13	a	63.80	0.33920	YES	YES
14	a	76.09	0.46646	YES	YES
15	a	82.01	0.53374	YES	YES
16	a	87.47	0.05751	YES	YES
17	a	95.81	0.15715	YES	YES
18	a	101.62	0.38770	YES	YES
19	a	121.65	0.62825	YES	YES
20	a	133.09	0.95562	YES	YES
21	a	158.91	0.65598	YES	YES
22	a	171.28	2.93053	YES	YES
23	a	204.45	8.52771	YES	YES
24	a	221.24	1.12574	YES	YES
25	a	225.57	2.57217	YES	YES
26	a	260.72	3.30447	YES	YES
27	a	262.54	0.90363	YES	YES
28	a	291.03	1.30239	YES	YES
29	a	312.22	11.28529	YES	YES
30	a	400.73	1.19342	YES	YES
31	a	405.42	0.45457	YES	YES
32	a	407.19	1.70779	YES	YES
33	a	420.52	2.13785	YES	YES
34	a	443.09	0.05262	YES	YES
35	a	445.72	2.31478	YES	YES
36	a	454.94	1.77653	YES	YES
37	a	468.28	3.39004	YES	YES
38	a	476.13	8.41032	YES	YES
39	a	481.68	2.49903	YES	YES
40	a	505.35	3.70312	YES	YES
41	a	515.80	16.83659	YES	YES
42	a	529.78	2.98947	YES	YES
43	a	534.51	2.41560	YES	YES
44	a	557.25	0.74365	YES	YES
45	a	569.79	5.61717	YES	YES
46	a	587.36	23.70126	YES	YES
47	a	610.02	1.28155	YES	YES
48	a	613.01	5.13310	YES	YES
49	a	618.55	45.97154	YES	YES
50	a	622.16	29.74323	YES	YES

3ha'

SCF Energy (au) BP86/SV(P) -2354.891997893
SCF Energy (au) PBE0/def2-TZVPP -2354.444420890
SCF Energy (au) PBE0/def2-TZVPP -2354.4536324230 (Toluene Correction)
Zero Point Energy (au) 0.3244849
Chemical Potential (kJ mol^{-1}) 697.48
Dispersion Correction (au) PBE0/def2-TZVPP -0.06855975

xyz coordinates
45

Mn	2.1473163	1.8360644	0.6549980
C	2.5134529	2.0827923	2.4407545
C	3.8276642	1.3205676	0.2474063
C	2.5110158	3.4912763	0.2106829
O	2.7127039	4.5988164	-0.1110798
O	4.9051974	0.9874349	-0.0456415
O	2.7825573	2.2571479	3.5616359
C	-0.5045838	1.0098222	1.1597239
C	0.3466433	-0.2156809	1.2987456
C	1.1533074	-0.6772435	0.2074169
C	1.9544921	-1.8298941	0.4274221
C	1.9730232	-2.4927127	1.6587154
C	1.1679062	-2.0335724	2.7208425
C	0.3570502	-0.9098951	2.5354940
H	2.5671394	-2.2034856	-0.4090707
H	2.6173836	-3.3767309	1.7954675
H	1.1768314	-2.5529085	3.6928652
H	-0.2797052	-0.5454997	3.3581044
N	0.1784474	2.0822057	0.8741866
H	1.7080949	1.7931007	-2.1537943
C	1.6406430	1.2400589	-1.1978645
C	1.1492211	-0.0302570	-1.1595934
C	0.6810864	-0.8366841	-2.3202024
C	-0.2729277	-2.3459176	-4.5442658
C	-0.6369745	-2.7028301	-3.2354055
C	-0.1647223	-1.9605573	-2.1409611
C	1.0454677	-0.4997397	-3.6491124
C	0.5730529	-1.2384981	-4.7421129
H	-0.6385616	-2.9299659	-5.4049812
H	-1.2979833	-3.5687365	-3.0615359
H	-0.4650140	-2.2553027	-1.1216221
H	1.7269371	0.3483022	-3.8237653
H	0.8789089	-0.9536970	-5.7629458
H	-0.3637364	2.9429415	0.7029938
C	-1.9679026	0.9717771	1.3689105
C	-4.7780709	0.8918705	1.7096646
C	-4.0775780	2.0974632	1.9001518
C	-2.6873017	2.1379152	1.7336900
C	-2.6839578	-0.2379989	1.1945194
C	-4.0764003	-0.2743310	1.3580252
H	-5.8718745	0.8613632	1.8428671
H	-4.6189613	3.0118872	2.1929712
H	-2.1503338	3.0831105	1.9209199
H	-2.1398434	-1.1520296	0.9082756
H	-4.6191108	-1.2217489	1.2065037

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.54	0.06232	YES	YES
8	a	30.72	0.02671	YES	YES
9	a	33.19	0.15313	YES	YES
10	a	35.77	0.03630	YES	YES
11	a	45.96	0.10263	YES	YES
12	a	48.02	0.04022	YES	YES
13	a	70.48	0.39725	YES	YES
14	a	74.21	0.99841	YES	YES
15	a	80.25	0.36004	YES	YES
16	a	82.52	0.06077	YES	YES
17	a	88.33	0.24855	YES	YES
18	a	98.18	0.28632	YES	YES
19	a	118.70	0.07417	YES	YES
20	a	139.85	0.35431	YES	YES
21	a	159.69	2.51650	YES	YES
22	a	180.91	1.89325	YES	YES
23	a	188.41	0.83797	YES	YES
24	a	202.24	0.22099	YES	YES
25	a	238.03	1.15483	YES	YES
26	a	272.89	5.68818	YES	YES
27	a	279.98	3.23812	YES	YES
28	a	299.79	0.96235	YES	YES
29	a	311.67	1.93608	YES	YES
30	a	399.61	0.79350	YES	YES
31	a	401.93	0.55369	YES	YES
32	a	405.62	1.29219	YES	YES
33	a	411.42	4.36505	YES	YES
34	a	448.49	2.32542	YES	YES
35	a	454.57	0.33329	YES	YES
36	a	462.84	0.31148	YES	YES
37	a	464.29	11.86901	YES	YES
38	a	473.01	1.22050	YES	YES
39	a	481.32	7.29869	YES	YES
40	a	509.53	3.69401	YES	YES
41	a	516.36	36.11068	YES	YES
42	a	528.45	2.40935	YES	YES
43	a	551.04	3.74614	YES	YES
44	a	572.47	7.19075	YES	YES
45	a	576.98	21.92925	YES	YES
46	a	607.33	4.65353	YES	YES
47	a	609.16	12.77565	YES	YES
48	a	611.63	38.74875	YES	YES
49	a	614.73	0.08764	YES	YES
50	a	621.80	51.19677	YES	YES

3ia

SCF Energy (au) BP86/SV(P) -2183.142508002
SCF Energy (au) PBE0/def2-TZVPP -2182.728425547
SCF Energy (au) PBE0/def2-TZVPP -2182.7357796019 (Toluene Correction)
Zero Point Energy (au) 0.2600039
Chemical Potential (kJ mol^{-1}) 539.07
Dispersion Correction (au) PBE0/def2-TZVPP -0.05212511

xyz coordinates
37

Mn	1.1217044	1.2220039	0.8753182
C	1.8076113	1.3348070	2.5749408
C	2.7421494	1.2108299	0.1355115
C	1.0314197	2.9638585	0.6742824
O	0.9561462	4.1202638	0.5160197
O	3.8034237	1.1815147	-0.3512306
O	2.2450875	1.3934439	3.6532134
C	-1.4143192	0.1032722	1.9810110
C	-2.7959384	0.3246958	2.5515022
C	-0.8039152	-1.2334355	1.9498273
C	0.0519542	-1.6099950	0.8541980
C	0.6098266	-2.9207387	0.9125915
C	0.3739047	-3.7930724	1.9771542
C	-0.4827170	-3.4144254	3.0316683
C	-1.0800704	-2.1522323	2.9934884
H	1.2462492	-3.2504250	0.0744264
H	0.8490304	-4.7880668	1.9802317
H	-0.6839061	-4.1018357	3.8684900
H	-1.7572007	-1.8499947	3.8081085
O	-0.7925239	1.0949317	1.5367526
C	0.2629736	0.8812582	-2.1683061
C	0.9689452	2.0137198	-2.6526610
C	0.8763286	2.4070638	-3.9944473
C	0.0527202	1.6977131	-4.8871522
C	-0.6794746	0.5894331	-4.4235589
C	-0.5752960	0.1877177	-3.0853985
H	1.6024832	2.5887464	-1.9605507
H	1.4454542	3.2836622	-4.3459625
H	-0.0297790	2.0165111	-5.9395503
H	-1.3430462	0.0381636	-5.1108464
H	-1.1711905	-0.6675105	-2.7248941
C	0.3562945	0.4549763	-0.7681487
C	0.2344433	-0.8812744	-0.4193629
H	0.4020035	-1.6010875	-1.2503389
H	-3.1358146	1.3486402	2.2980282
H	-2.7730963	0.2339713	3.6619155
H	-3.5218654	-0.4271045	2.1737291

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.40	2.54394	YES	YES
8	a	24.72	0.10778	YES	YES
9	a	43.63	1.36218	YES	YES
10	a	54.12	0.02016	YES	YES

11	a	60.67	0.24551	YES	YES
12	a	72.56	0.62244	YES	YES
13	a	79.27	0.63032	YES	YES
14	a	90.97	0.49506	YES	YES
15	a	95.26	0.11903	YES	YES
16	a	101.74	0.77547	YES	YES
17	a	111.63	1.15725	YES	YES
18	a	125.72	0.08378	YES	YES
19	a	152.51	0.33523	YES	YES
20	a	169.52	8.67190	YES	YES
21	a	192.37	0.29482	YES	YES
22	a	216.20	10.12995	YES	YES
23	a	232.41	0.24448	YES	YES
24	a	241.88	0.75526	YES	YES
25	a	252.52	6.68820	YES	YES
26	a	293.90	4.90373	YES	YES
27	a	353.55	2.36095	YES	YES
28	a	392.82	1.60206	YES	YES
29	a	406.09	0.60766	YES	YES
30	a	416.38	3.11805	YES	YES
31	a	431.45	0.83475	YES	YES
32	a	452.00	0.63243	YES	YES
33	a	467.01	0.40503	YES	YES
34	a	474.57	3.83516	YES	YES
35	a	487.49	12.99325	YES	YES
36	a	493.95	0.21123	YES	YES
37	a	520.07	1.81214	YES	YES
38	a	527.15	5.65477	YES	YES
39	a	533.50	0.52258	YES	YES
40	a	564.99	3.57873	YES	YES
41	a	579.71	0.36755	YES	YES
42	a	600.52	1.20567	YES	YES
43	a	611.17	1.41382	YES	YES
44	a	612.98	25.26251	YES	YES
45	a	621.48	7.53164	YES	YES
46	a	629.58	25.23277	YES	YES
47	a	645.56	30.57528	YES	YES
48	a	688.43	28.37147	YES	YES
49	a	697.66	30.34196	YES	YES
50	a	717.08	11.57712	YES	YES

3ia'

SCF Energy (au) BP86/SV(P) -2183.136961706
SCF Energy (au) PBE0/def2-TZVPP -2182.727556389
SCF Energy (au) PBE0/def2-TZVPP -2182.7350096537 (Toluene Correction)
Zero Point Energy (au) 0.2598973
Chemical Potential (kJ mol^{-1}) 537.84
Dispersion Correction (au) PBE0/def2-TZVPP -0.05187819

xyz coordinates
37

Mn	1.1456731	2.4084287	1.0514434
C	1.2843480	3.0374348	2.7773269
C	2.8931301	2.1414828	0.8561337
C	1.3131216	4.0054815	0.3609113
O	1.3955239	5.0598688	-0.1377030
O	4.0299225	1.9255071	0.7060206
O	1.4135291	3.4230247	3.8688410
C	-1.5463574	1.2579627	1.3745898
C	-3.0483446	1.3691686	1.4009870
C	-0.8895210	-0.0592515	1.6022068
C	0.0720327	-0.5659509	0.6705188
C	0.6462642	-1.8285391	0.9599993
C	0.3247948	-2.5445601	2.1197813
C	-0.6257246	-2.0367553	3.0241373
C	-1.2423982	-0.8112986	2.7495235
H	1.3697638	-2.2486436	0.2426544
H	0.8152544	-3.5120111	2.3177643
H	-0.8882081	-2.5966910	3.9362526
H	-1.9917681	-0.4121785	3.4530209
O	-0.8668938	2.2793093	1.1438564
H	1.1975253	1.7970538	-1.6421925
C	0.9189164	1.4000598	-0.6460373
C	0.4425086	0.1143609	-0.6185621
C	0.3414973	-0.7211797	-1.8562369
H	-3.3556380	2.4322364	1.3398434
H	-3.4756974	0.9006292	2.3143817
H	-3.4705582	0.8113526	0.5333939
C	0.0811686	-2.2377162	-4.2519088
C	-0.8457575	-2.3966710	-3.2071173
C	-0.7134116	-1.6537369	-2.0239658
C	1.2731481	-0.5851976	-2.9146930
C	1.1430398	-1.3293998	-4.0968532
H	-0.0187059	-2.8250778	-5.1797095
H	-1.6839069	-3.1057620	-3.3152054
H	-1.4534085	-1.7869382	-1.2170713
H	2.1270325	0.1014893	-2.7953285
H	1.8881048	-1.2072921	-4.9010036

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.03	0.04299	YES	YES
8	a	29.88	0.03834	YES	YES
9	a	43.82	0.16594	YES	YES
10	a	51.24	0.15359	YES	YES

11	a	61.74	0.30398	YES	YES
12	a	69.23	1.44302	YES	YES
13	a	79.86	0.04878	YES	YES
14	a	85.57	0.38966	YES	YES
15	a	88.81	0.11878	YES	YES
16	a	97.83	0.27936	YES	YES
17	a	106.39	0.50957	YES	YES
18	a	110.87	0.22317	YES	YES
19	a	146.59	2.94774	YES	YES
20	a	157.49	1.94876	YES	YES
21	a	204.75	0.39131	YES	YES
22	a	218.92	2.28317	YES	YES
23	a	231.59	0.37369	YES	YES
24	a	252.43	0.43101	YES	YES
25	a	289.71	0.21352	YES	YES
26	a	309.83	0.54719	YES	YES
27	a	358.37	0.71677	YES	YES
28	a	374.94	1.21258	YES	YES
29	a	404.39	0.02014	YES	YES
30	a	417.18	2.72831	YES	YES
31	a	427.00	1.39593	YES	YES
32	a	445.95	1.88235	YES	YES
33	a	457.11	1.40503	YES	YES
34	a	465.73	7.32504	YES	YES
35	a	486.02	2.33309	YES	YES
36	a	521.44	4.72483	YES	YES
37	a	523.49	5.61477	YES	YES
38	a	527.41	4.31855	YES	YES
39	a	547.92	4.01688	YES	YES
40	a	577.62	2.23764	YES	YES
41	a	598.63	2.96917	YES	YES
42	a	599.31	11.79126	YES	YES
43	a	612.20	1.68466	YES	YES
44	a	614.93	32.37495	YES	YES
45	a	618.76	29.53671	YES	YES
46	a	630.83	8.60057	YES	YES
47	a	657.53	6.90263	YES	YES
48	a	695.80	27.47499	YES	YES
49	a	696.46	8.46114	YES	YES
50	a	704.54	39.55734	YES	YES

3ja

SCF Energy (au) BP86/SV(P)	-2452.103080854
SCF Energy (au) PBE0/def2-TZVPP	-2451.641880652
SCF Energy (au) PBE0/def2-TZVPP	-2451.6499605316 (Toluene Correction)
Zero Point Energy (au)	0.3448731
Chemical Potential (kJ mol^{-1})	740.54
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06861384

xyz coordinates

48

Mn	1.6497721	1.3358800	0.5377851
C	2.2607111	1.1039574	2.2578338
C	3.2884896	1.2193251	-0.1490047
C	1.7869671	3.0934275	0.5737376
O	1.8781603	4.2597576	0.5697864
O	4.3558709	1.1265886	-0.6172802
O	2.6536735	0.9511328	3.3429371
C	-1.0368873	0.4731728	1.4794316
C	-2.3887641	0.7350323	2.0440928
C	-0.4926578	-0.8470109	1.3727270
C	0.4605652	-1.1886026	0.3999303
C	1.0481149	-2.5666603	0.4574499
O	-0.3496116	1.4707664	1.0859053
C	0.6702105	1.4277704	-2.5020987
C	1.2395772	2.6775180	-2.8692160
C	1.0967138	3.1776742	-4.1690384
C	0.3650077	2.4529686	-5.1285574
C	-0.2254533	1.2226328	-4.7807425
C	-0.0754722	0.7160695	-3.4848411
H	1.7947466	3.2520937	-2.1120276
H	1.5514070	4.1454229	-4.4374168
H	0.2445661	2.8532503	-6.1490767
H	-0.8099279	0.6599920	-5.5274730
H	-0.5511774	-0.2390094	-3.2066295
C	0.8194577	0.9109833	-1.1540798
C	0.7721341	-0.4483760	-0.8194785
H	1.1284006	-1.1315150	-1.6198489
H	-0.8315661	-1.6271544	2.0700320
C	2.2169575	-5.1499094	0.5825091
C	2.9898023	-4.0412065	0.1967011
C	2.4100757	-2.7654005	0.1272300
C	0.2826793	-3.6927490	0.8410522
C	0.8598144	-4.9705594	0.8999324
H	2.6713797	-6.1531857	0.6332252
H	4.0574584	-4.1677738	-0.0476822
H	3.0296920	-1.8999209	-0.1607391
H	-0.7895347	-3.5740838	1.0665908
H	0.2402736	-5.8351928	1.1902115
C	-4.9417765	1.3110561	3.1085565
C	-4.5833454	-0.0176796	2.8192199
C	-3.3178408	-0.3043725	2.2870562
C	-2.7625783	2.0690374	2.3354150
C	-4.0287738	2.3534290	2.8623771
H	-5.9378888	1.5353865	3.5250813
H	-5.2993217	-0.8358795	3.0019444
H	-3.0572988	-1.3454709	2.0391041
H	-2.0348341	2.8714214	2.1397768
H	-4.3079682	3.3959661	3.0875984

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.61	0.38846	YES	YES
8	a	22.13	1.40826	YES	YES
9	a	29.62	0.58524	YES	YES
10	a	35.83	0.11973	YES	YES
11	a	37.15	1.03095	YES	YES
12	a	45.28	0.39974	YES	YES
13	a	51.69	0.80298	YES	YES
14	a	53.97	0.16678	YES	YES
15	a	59.96	0.19192	YES	YES
16	a	83.78	0.20446	YES	YES
17	a	88.78	0.11842	YES	YES
18	a	94.65	0.05377	YES	YES
19	a	108.34	1.43645	YES	YES
20	a	112.52	0.66592	YES	YES
21	a	121.74	2.50328	YES	YES
22	a	137.87	2.51867	YES	YES
23	a	154.04	1.13695	YES	YES
24	a	159.72	19.21260	YES	YES
25	a	208.77	5.50424	YES	YES
26	a	223.45	5.51475	YES	YES
27	a	236.61	6.29007	YES	YES
28	a	244.48	0.51186	YES	YES
29	a	263.63	0.36410	YES	YES
30	a	300.33	15.23751	YES	YES
31	a	315.45	2.35486	YES	YES
32	a	354.74	4.40350	YES	YES
33	a	399.79	0.34017	YES	YES
34	a	401.89	0.37964	YES	YES
35	a	404.00	0.99737	YES	YES
36	a	410.72	1.43291	YES	YES
37	a	432.02	13.66021	YES	YES
38	a	444.42	0.94919	YES	YES
39	a	449.20	0.88613	YES	YES
40	a	469.99	3.80862	YES	YES
41	a	476.01	1.14658	YES	YES
42	a	490.75	5.89549	YES	YES
43	a	511.19	3.28314	YES	YES
44	a	523.69	2.96840	YES	YES
45	a	532.69	13.34996	YES	YES
46	a	537.60	6.45739	YES	YES
47	a	571.53	10.37027	YES	YES
48	a	595.22	21.30454	YES	YES
49	a	600.42	1.13653	YES	YES
50	a	609.38	0.96738	YES	YES

8ia

SCF Energy (au) BP86/SV(P) -2183.167100726
SCF Energy (au) PBE0/def2-TZVPP -2182.760093970
SCF Energy (au) PBE0/def2-TZVPP -2182.7673435546 (Toluene Correction)
Zero Point Energy (au) 0.262048
Chemical Potential (kJ mol^{-1}) 552.88
Dispersion Correction (au) PBE0/def2-TZVPP -0.05528328

xyz coordinates
37

C	0.5519872	-2.6912867	-1.2913389
C	0.2840276	-0.7130500	-2.8426551
C	-0.3152585	0.3674579	-0.0427651
C	2.6292711	-1.3094929	-1.9255555
C	-1.1180588	-1.5613016	1.0385935
C	-1.8861600	-2.6710730	1.4213656
C	-0.5344483	-2.8386193	3.4524914
C	0.2436599	-1.7263580	3.0576751
C	-0.0589658	-1.0903227	1.8545506
C	0.6506036	0.0699627	1.1437708
C	1.0179321	1.2176860	2.0832109
Mn	1.0064560	-0.9825830	-1.2152724
O	1.7826055	-0.4273318	0.4228709
O	0.2895606	-3.8286872	-1.2814776
O	-0.1846590	-0.4983389	-3.8894827
C	-1.1895038	-0.7156615	-0.1640049
O	3.6722692	-1.5186156	-2.3927036
C	-1.5874721	-3.3030468	2.6447767
H	-1.9587835	-0.8286218	-0.9438598
C	-0.2589714	1.5834644	-0.8799974
C	-0.2088766	3.9319931	-2.4783775
C	0.9676993	3.4679743	-1.8653119
C	0.9489654	2.3093202	-1.0758683
C	-1.4363562	2.0636611	-1.5112907
C	-1.4104639	3.2233530	-2.2967212
H	-0.1902141	4.8431914	-3.0984616
H	1.9172306	4.0091726	-2.0092557
H	1.8825905	1.9313140	-0.6341402
H	-2.3891518	1.5325110	-1.3564038
H	-2.3404965	3.5823853	-2.7675948
H	1.0743472	-1.3783058	3.6934000
H	-0.3103288	-3.3497958	4.4034055
H	-2.1830567	-4.1722517	2.9692037
H	-2.7093477	-3.0381332	0.7864306
H	1.4649868	2.0723840	1.5358923
H	1.7650006	0.8569529	2.8231957
H	0.1213801	1.5800935	2.6317052

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.11	0.20072	YES	YES
8	a	43.70	0.18262	YES	YES
9	a	55.91	0.39403	YES	YES
10	a	72.01	0.02060	YES	YES

11	a	78.66	0.27668	YES	YES
12	a	86.20	0.40743	YES	YES
13	a	91.56	0.15210	YES	YES
14	a	99.13	0.43175	YES	YES
15	a	106.62	0.83380	YES	YES
16	a	108.75	0.38617	YES	YES
17	a	124.81	0.80891	YES	YES
18	a	173.83	1.02082	YES	YES
19	a	187.33	0.44146	YES	YES
20	a	208.12	0.11055	YES	YES
21	a	236.87	0.28880	YES	YES
22	a	250.26	0.29553	YES	YES
23	a	262.29	2.69722	YES	YES
24	a	276.55	0.22091	YES	YES
25	a	311.10	7.63204	YES	YES
26	a	335.74	4.50892	YES	YES
27	a	358.90	3.92761	YES	YES
28	a	409.49	0.48452	YES	YES
29	a	415.74	1.38512	YES	YES
30	a	441.65	6.35928	YES	YES
31	a	449.05	0.51048	YES	YES
32	a	464.02	4.18320	YES	YES
33	a	477.83	10.23579	YES	YES
34	a	484.00	5.78995	YES	YES
35	a	503.35	9.08164	YES	YES
36	a	521.28	8.94887	YES	YES
37	a	532.86	1.55631	YES	YES
38	a	556.82	8.49744	YES	YES
39	a	560.73	5.82532	YES	YES
40	a	590.10	10.15338	YES	YES
41	a	599.96	27.22976	YES	YES
42	a	607.28	14.07331	YES	YES
43	a	610.71	3.00172	YES	YES
44	a	638.06	18.14658	YES	YES
45	a	648.93	20.96493	YES	YES
46	a	670.45	18.26347	YES	YES
47	a	692.11	31.38006	YES	YES
48	a	697.96	21.35305	YES	YES
49	a	704.56	12.89033	YES	YES
50	a	746.65	33.45622	YES	YES

8ja

SCF Energy (au) BP86/SV(P)		-2452.112960024
SCF Energy (au) PBE0/def2-TZVPP		-2451.661992594
SCF Energy (au) PBE0/def2-TZVPP		-2451.6706401152 (Toluene Correction)
Zero Point Energy (au)		0.3460163
Chemical Potential (kJ mol^{-1})		747.33
Dispersion Correction (au)	PBE0/def2-TZVPP	-0.07305111

xyz coordinates
48

C	0.8108323	-2.5903869	-1.8551545
C	0.3540829	-0.6479745	-3.4094316
C	-0.0826625	0.4169862	-0.5404790
C	2.7762166	-1.1195163	-2.6223677
C	-0.8478166	-1.4866598	0.6328914
C	-1.7366531	-2.6171487	0.9565024
C	0.2389347	-1.0390112	1.3320947
C	0.9318723	0.0981200	0.5907915
C	1.3462114	1.2268378	1.5268983
Mn	1.1834611	-0.8643311	-1.8247111
O	2.0238398	-0.4190367	-0.1702391
O	0.6133847	-3.7407970	-1.8329725
O	-0.1845942	-0.4812006	-4.4314630
C	-0.9733815	-0.6514769	-0.5916826
O	3.8052897	-1.2837979	-3.1362321
H	-1.7905066	-0.7560741	-1.3207365
C	-0.0049395	1.6024817	-1.4098848
C	0.1173724	3.9102760	-3.0585552
C	1.2408968	3.5139527	-2.3143373
C	1.1863709	2.3767047	-1.4952047
C	-1.1333642	2.0200555	-2.1687061
C	-1.0715674	3.1590736	-2.9776495
H	0.1631612	4.8064150	-3.6988284
H	2.1747461	4.0968736	-2.3679992
H	2.0717122	2.0692665	-0.9211398
H	-2.0760080	1.4540942	-2.0993076
H	-1.9618472	3.4706015	-3.5482432
C	-3.4330047	-4.8051935	1.5919634
C	-2.6637013	-4.1884179	2.5962573
C	-1.8294188	-3.1077696	2.2832143
C	-2.5224466	-3.2442275	-0.0407170
C	-3.3575429	-4.3279362	0.2732583
H	-4.0918794	-5.6539004	1.8389797
H	-2.7208029	-4.5500213	3.6363777
H	-1.2500667	-2.6188642	3.0831149
H	-2.4615598	-2.9022017	-1.0859113
H	-3.9514708	-4.8057075	-0.5233034
C	2.1262996	3.2434620	3.3417805
C	3.0871860	2.3796812	2.7891985
C	2.7002511	1.3750198	1.8854352
C	0.3845893	2.0930841	2.0859939
C	0.7729370	3.0974656	2.9870120
H	2.4308740	4.0329286	4.0488730
H	4.1503046	2.4888908	3.0619363
H	3.4429536	0.6954052	1.4389028
H	-0.6785673	1.9830107	1.8118488
H	0.0129662	3.7725691	3.4145818
H	0.6770557	-1.4816048	2.2373501

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.39	0.51363	YES	YES
8	a	32.12	0.20469	YES	YES
9	a	34.81	0.10117	YES	YES
10	a	37.44	0.46825	YES	YES
11	a	40.24	0.01493	YES	YES
12	a	45.91	0.16691	YES	YES
13	a	51.66	0.12131	YES	YES
14	a	67.30	0.24290	YES	YES
15	a	73.61	0.08827	YES	YES
16	a	82.74	0.23275	YES	YES
17	a	90.31	0.58714	YES	YES
18	a	96.41	0.25560	YES	YES
19	a	106.21	1.03310	YES	YES
20	a	122.44	0.07124	YES	YES
21	a	135.04	0.29045	YES	YES
22	a	159.90	0.70650	YES	YES
23	a	171.85	2.70924	YES	YES
24	a	202.85	1.28940	YES	YES
25	a	216.36	0.94684	YES	YES
26	a	226.97	1.21257	YES	YES
27	a	240.13	3.80695	YES	YES
28	a	258.11	1.61148	YES	YES
29	a	265.91	0.05346	YES	YES
30	a	335.01	4.01898	YES	YES
31	a	383.95	0.80238	YES	YES
32	a	401.10	0.41059	YES	YES
33	a	401.14	0.52167	YES	YES
34	a	404.62	0.48174	YES	YES
35	a	412.48	2.77429	YES	YES
36	a	420.42	1.67771	YES	YES
37	a	443.53	7.46887	YES	YES
38	a	450.80	1.71787	YES	YES
39	a	466.08	11.60292	YES	YES
40	a	472.43	5.63197	YES	YES
41	a	480.54	4.86212	YES	YES
42	a	497.71	15.38443	YES	YES
43	a	512.43	20.50597	YES	YES
44	a	531.11	2.32273	YES	YES
45	a	542.35	12.22692	YES	YES
46	a	563.25	9.03231	YES	YES
47	a	599.68	11.71928	YES	YES
48	a	604.55	11.06808	YES	YES
49	a	609.38	3.49552	YES	YES
50	a	610.81	2.20605	YES	YES

9ia

SCF Energy (au) BP86/SV(P) -2183.138380453
SCF Energy (au) PBE0/def2-TZVPP -2182.724742562
SCF Energy (au) PBE0/def2-TZVPP -2182.7310254792 (Toluene Correction)
Zero Point Energy (au) 0.2609739
Chemical Potential (kJ mol^{-1}) 548.90
Dispersion Correction (au) PBE0/def2-TZVPP -0.05007606

xyz coordinates
37

C	-0.4555222	-1.0272451	3.0134137
C	-2.2322748	0.4111283	1.9710883
C	0.0765045	0.6592913	0.2153566
C	-2.0328828	-2.2131014	1.3040033
C	0.6943673	-1.7017693	0.2059772
C	1.4316334	-2.8323304	0.7623819
C	1.3005899	-4.0080826	-1.3831930
C	0.5988639	-2.9877527	-1.9733225
C	0.2029760	-1.8214566	-1.2085885
C	-0.5734114	-0.7912101	-1.6547933
C	-1.1030889	-0.4177771	-2.9922619
Mn	-0.9860359	-0.7326150	1.3497814
O	-0.9747193	0.1184265	-0.6077278
O	-0.0663219	-1.2180463	4.0996646
O	-3.0346241	1.1523496	2.3770901
C	0.9524247	-0.3565723	0.6718398
O	-2.7078744	-3.1600726	1.2635249
C	1.7089756	-3.9403243	0.0073344
H	1.7758198	-0.1248679	1.3632294
C	0.1894817	2.1233550	0.2802081
C	0.3726487	4.9465356	0.4286199
C	-0.6867555	4.3411891	-0.2687163
C	-0.7816514	2.9441210	-0.3418260
C	1.2592495	2.7430561	0.9719089
C	1.3436830	4.1395897	1.0490001
H	0.4435155	6.0448941	0.4884125
H	-1.4530753	4.9637220	-0.7593994
H	-1.6178905	2.4722011	-0.8791882
H	2.0349144	2.1291004	1.4564324
H	2.1816553	4.6031950	1.5951619
H	0.2850503	-3.0663822	-3.0270335
H	1.5562552	-4.9047089	-1.9718040
H	2.2602328	-4.7868424	0.4477199
H	1.7740923	-2.7639756	1.8084347
H	-0.8191214	-1.1743746	-3.7523658
H	-0.7027317	0.5686405	-3.3272306
H	-2.2149523	-0.3312879	-2.9831333

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	32.09	0.16433	YES	YES
8	a	41.04	0.43457	YES	YES
9	a	43.30	0.08549	YES	YES
10	a	61.32	0.14316	YES	YES

11	a	70.63	0.24433	YES	YES
12	a	80.44	0.10310	YES	YES
13	a	88.72	0.56643	YES	YES
14	a	91.28	0.09064	YES	YES
15	a	101.03	0.17071	YES	YES
16	a	122.69	0.88529	YES	YES
17	a	137.08	0.61744	YES	YES
18	a	154.22	0.07845	YES	YES
19	a	160.24	2.97304	YES	YES
20	a	194.72	3.09354	YES	YES
21	a	210.73	1.39781	YES	YES
22	a	225.33	0.10436	YES	YES
23	a	264.83	0.46515	YES	YES
24	a	279.37	0.16220	YES	YES
25	a	328.31	2.31572	YES	YES
26	a	395.22	2.39126	YES	YES
27	a	401.33	1.58970	YES	YES
28	a	416.82	3.66140	YES	YES
29	a	423.99	7.52465	YES	YES
30	a	435.17	1.33824	YES	YES
31	a	461.94	5.83288	YES	YES
32	a	464.69	8.61675	YES	YES
33	a	473.03	2.00337	YES	YES
34	a	483.39	4.12031	YES	YES
35	a	485.54	1.74401	YES	YES
36	a	499.73	10.17819	YES	YES
37	a	505.07	2.18928	YES	YES
38	a	525.63	10.68491	YES	YES
39	a	528.37	6.68453	YES	YES
40	a	539.64	8.83679	YES	YES
41	a	569.83	17.33705	YES	YES
42	a	606.92	22.91671	YES	YES
43	a	609.38	19.50509	YES	YES
44	a	615.44	28.65066	YES	YES
45	a	639.94	47.13741	YES	YES
46	a	648.67	22.80887	YES	YES
47	a	677.37	47.26649	YES	YES
48	a	690.85	40.63817	YES	YES
49	a	700.88	5.60458	YES	YES
50	a	705.66	7.87861	YES	YES

9ja

SCF Energy (au) BP86/SV(P)		-2452.123348709
SCF Energy (au) PBE0/def2-TZVPP		-2451.669527954
SCF Energy (au) PBE0/def2-TZVPP		-2451.6778817812 (Toluene Correction)
Zero Point Energy (au)		0.3465202
Chemical Potential (kJ mol^{-1})		748.52
Dispersion Correction (au)	PBE0/def2-TZVPP	-0.06711919

xyz coordinates
48

C	2.3481734	2.2431881	1.1948046
C	0.1669204	2.3188157	2.4292183
C	-0.4497452	1.1219581	-0.1618083
C	1.7887959	0.1560994	2.6481949
C	1.5063152	-0.3478334	-0.2672712
C	2.9328444	-0.6229345	-0.5999385
C	0.5954253	-1.4898840	-0.0218430
C	-0.6543657	-1.2326713	0.4334046
C	-1.8283792	-2.0885233	0.5937571
Mn	0.9803039	1.1277700	1.3506333
O	-0.8371988	0.1422389	0.8244142
O	3.2417433	2.9837327	1.0599128
O	-0.3559810	3.0919240	3.1280260
C	0.8256757	0.8453429	-0.7168583
O	2.3032906	-0.4872383	3.4703845
H	1.2711844	1.5624460	-1.4211007
C	-1.4756507	2.0835584	-0.5975933
C	-4.0855982	-3.7748885	0.9452271
C	-2.9467578	-4.2450724	0.2634206
C	-1.8353585	-3.4137417	0.0830389
C	-2.9808622	-1.6281341	1.2788312
C	-4.0956897	-2.4630130	1.4475238
H	-4.9620109	-4.4296990	1.0795436
H	-2.9293074	-5.2697910	-0.1430840
H	-0.9636572	-3.7922900	-0.4742328
H	-2.9923089	-0.6067439	1.6857237
H	-4.9814458	-2.0831672	1.9829698
H	0.8987698	-2.5058650	-0.3135795
C	-3.4319440	3.9575317	-1.4261029
C	-2.3158747	3.6942575	-2.2390909
C	-1.3504676	2.7605723	-1.8347964
C	-2.6048486	2.3545139	0.2113516
C	-3.5729147	3.2799432	-0.2017181
H	-4.1933155	4.6868346	-1.7478189
H	-2.2010025	4.2109463	-3.2061260
H	-0.4983866	2.5433499	-2.4980973
H	-2.7102842	1.8425986	1.1795225
H	-4.4441656	3.4791372	0.4434947
C	5.6523835	-1.2186915	-1.2127869
C	5.0527270	-0.0436213	-1.6970863
C	3.7148678	0.2504861	-1.3942853
C	3.5578032	-1.7978579	-0.1128142
C	4.8955628	-2.0926406	-0.4142897
H	6.7043340	-1.4473057	-1.4498788
H	5.6332163	0.6573574	-2.3196217
H	3.2815708	1.1826469	-1.7890620
H	2.9934402	-2.4831364	0.5401539
H	5.3521732	-3.0125058	-0.0126667

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.18	0.33573	YES	YES
8	a	25.47	0.04866	YES	YES
9	a	28.98	0.47989	YES	YES
10	a	37.98	0.33424	YES	YES
11	a	40.14	0.15511	YES	YES
12	a	43.28	0.33799	YES	YES
13	a	47.51	0.07398	YES	YES
14	a	64.19	0.02483	YES	YES
15	a	65.43	0.04008	YES	YES
16	a	85.18	0.26396	YES	YES
17	a	86.74	0.47070	YES	YES
18	a	99.55	0.10688	YES	YES
19	a	112.34	0.21166	YES	YES
20	a	133.07	0.22799	YES	YES
21	a	156.64	0.23988	YES	YES
22	a	176.24	0.31802	YES	YES
23	a	178.08	5.06385	YES	YES
24	a	201.08	1.21054	YES	YES
25	a	224.13	0.38223	YES	YES
26	a	231.65	0.53260	YES	YES
27	a	253.66	0.13913	YES	YES
28	a	283.75	0.39827	YES	YES
29	a	339.79	1.84763	YES	YES
30	a	370.05	0.66602	YES	YES
31	a	397.59	0.44885	YES	YES
32	a	399.17	1.01817	YES	YES
33	a	400.76	0.01344	YES	YES
34	a	409.24	6.36317	YES	YES
35	a	419.18	9.63843	YES	YES
36	a	429.06	3.29580	YES	YES
37	a	446.88	0.94191	YES	YES
38	a	454.75	2.00890	YES	YES
39	a	471.78	6.65950	YES	YES
40	a	475.15	4.60871	YES	YES
41	a	491.20	5.83447	YES	YES
42	a	497.32	7.85839	YES	YES
43	a	505.28	16.47287	YES	YES
44	a	529.69	11.38708	YES	YES
45	a	542.19	1.29025	YES	YES
46	a	556.07	1.17116	YES	YES
47	a	577.70	32.51701	YES	YES
48	a	594.52	11.60200	YES	YES
49	a	610.95	9.31423	YES	YES
50	a	611.61	15.19755	YES	YES

10ia

SCF Energy (au) BP86/SV(P) -2183.171667761
SCF Energy (au) PBE0/def2-TZVPP -2182.759271019
SCF Energy (au) PBE0/def2-TZVPP -2182.7662187626 (Toluene Correction)
Zero Point Energy (au) 0.2623685
Chemical Potential (kJ mol^{-1}) 552.90
Dispersion Correction (au) PBE0/def2-TZVPP -0.05036288

xyz coordinates
37

C	1.7416408	-0.3110429	2.6964122
C	-0.8712760	0.4193370	2.4633608
C	-0.1669048	0.7917484	-0.6034849
C	-0.1250551	-2.0260195	2.8690518
C	1.2989200	-1.1605016	-0.1507975
C	2.5785955	-1.7819943	-0.2919384
C	1.5068238	-3.9769796	-0.2672980
C	0.2492646	-3.4050117	-0.1216549
C	0.1094744	-1.9805270	-0.0721054
C	-1.0938021	-1.1981647	0.2068743
Mn	0.2702500	-0.7301946	1.7199400
O	-1.2283806	-0.0104199	-0.6625917
O	2.6724097	-0.0025099	3.3308564
O	-1.6464613	1.1574311	2.9338273
C	1.0636290	0.2867299	-0.1509372
O	-0.3985336	-2.8882566	3.6113264
C	2.6744766	-3.1661645	-0.3522813
H	1.9213850	0.9676776	-0.0641243
C	-0.4078879	2.1686693	-1.0679434
C	-0.9215874	4.8009094	-1.9518210
C	0.4022624	4.3317557	-1.8682576
C	0.6593036	3.0255458	-1.4329481
C	-1.7371538	2.6507631	-1.1584131
C	-1.9892911	3.9564387	-1.5985609
H	-1.1209938	5.8296381	-2.2948752
H	1.2405463	4.9881441	-2.1531103
H	1.6979338	2.6616762	-1.3974042
H	-2.5646823	1.9881558	-0.8651030
H	-3.0271132	4.3225561	-1.6596933
C	-2.4511310	-1.8280817	0.3522992
H	3.4786001	-1.1497834	-0.3651810
H	3.6626138	-3.6431160	-0.4562814
H	1.6052489	-5.0741229	-0.3131083
H	-0.6497154	-4.0382788	-0.0630405
H	-3.1796535	-1.0938172	0.7576642
H	-2.4062060	-2.6792928	1.0632910
H	-2.8475492	-2.2028965	-0.6219486

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	22.93	2.04808	YES	YES
8	a	35.63	0.05486	YES	YES
9	a	37.64	0.06628	YES	YES
10	a	67.71	1.08211	YES	YES

11	a	79.74	0.19435	YES	YES
12	a	83.10	0.33410	YES	YES
13	a	93.34	0.53032	YES	YES
14	a	98.58	0.34548	YES	YES
15	a	106.97	0.20771	YES	YES
16	a	132.40	2.84990	YES	YES
17	a	140.23	0.70162	YES	YES
18	a	150.70	0.84470	YES	YES
19	a	181.14	0.41538	YES	YES
20	a	207.09	0.50058	YES	YES
21	a	231.63	5.33756	YES	YES
22	a	262.88	0.13112	YES	YES
23	a	285.43	8.88123	YES	YES
24	a	299.28	0.21116	YES	YES
25	a	318.43	1.84098	YES	YES
26	a	327.54	4.75623	YES	YES
27	a	399.85	0.04054	YES	YES
28	a	416.07	4.37544	YES	YES
29	a	430.70	0.97133	YES	YES
30	a	433.74	7.94172	YES	YES
31	a	468.24	4.45534	YES	YES
32	a	469.79	6.79562	YES	YES
33	a	474.59	0.46909	YES	YES
34	a	489.99	3.20937	YES	YES
35	a	492.12	0.24457	YES	YES
36	a	506.72	8.96440	YES	YES
37	a	515.59	12.62066	YES	YES
38	a	527.61	7.60533	YES	YES
39	a	531.09	6.41458	YES	YES
40	a	559.16	2.49141	YES	YES
41	a	589.33	2.07303	YES	YES
42	a	607.23	29.54767	YES	YES
43	a	610.28	3.70786	YES	YES
44	a	639.55	48.54657	YES	YES
45	a	656.40	12.12776	YES	YES
46	a	660.05	24.40755	YES	YES
47	a	677.96	60.85678	YES	YES
48	a	686.84	36.23974	YES	YES
49	a	713.28	1.40244	YES	YES
50	a	728.90	69.19622	YES	YES

10ja

SCF Energy (au) BP86/SV(P)	-2452.145470468
SCF Energy (au) PBE0/def2-TZVPP	-2451.692028912
SCF Energy (au) PBE0/def2-TZVPP	-2451.7000699796 (Toluene Correction)
Zero Point Energy (au)	0.3474597
Chemical Potential (kJ mol^{-1})	755.51
Dispersion Correction (au) PBE0/def2-TZVPP	-0.06824413

xyz coordinates
48

C	1.6780743	1.2309898	1.9923960
C	-0.9898958	1.2615352	1.9040674
C	-0.0394979	1.1257232	-0.7683092
C	0.4310896	-0.8285674	2.7266545
C	1.3244149	-0.8822765	-0.2962105
C	0.0619891	-1.4838559	0.0472746
C	-1.1331050	-0.7307102	-0.1021554
Mn	0.3600532	0.2340567	1.2849380
O	-1.1312380	0.2895431	-1.0807702
O	2.5330402	1.8902683	2.4346122
O	-1.8603645	1.9235846	2.3016812
C	1.2333480	0.5092709	-0.6593866
O	0.4648208	-1.5390475	3.6535217
H	2.1524689	1.1048530	-0.7607071
C	-0.2579604	2.5575621	-1.0564700
C	-0.6966560	5.2882393	-1.6795272
C	0.5287824	4.8748054	-1.1231468
C	0.7465173	3.5273047	-0.8115288
C	-1.4886779	2.9853354	-1.6077039
C	-1.7022905	4.3375931	-1.9170142
H	-0.8671356	6.3509757	-1.9180002
H	1.3210578	5.6136587	-0.9187918
H	1.7011818	3.2340919	-0.3462086
H	-2.2783306	2.2436561	-1.7939022
H	-2.6684209	4.6501937	-2.3464741
C	-2.4754089	-1.2349964	0.2527769
C	2.6058982	-1.6329494	-0.3207534
H	0.0287655	-2.4999361	0.4664834
C	-5.0553649	-2.2494116	0.8431010
C	-3.9315986	-2.7098572	1.5552067
C	-2.6564172	-2.2072815	1.2680186
C	-3.6124354	-0.7720371	-0.4502200
C	-4.8886191	-1.2782083	-0.1573178
H	-6.0586393	-2.6424943	1.0759038
H	-4.0521713	-3.4610638	2.3530786
H	-1.7964039	-2.5563690	1.8618409
H	-3.4834345	-0.0170514	-1.2389274
H	-5.7620081	-0.9074773	-0.7189706
C	5.0466716	-3.0764760	-0.4370671
C	4.8041327	-2.0249083	-1.3355181
C	3.5947439	-1.3125070	-1.2801693
C	2.8643005	-2.6954262	0.5781829
C	4.0694764	-3.4087702	0.5196244
H	5.9948251	-3.6371283	-0.4799934
H	5.5581945	-1.7596333	-2.0948183
H	3.4034500	-0.5111931	-2.0121849
H	2.1258729	-2.9477113	1.3563622
H	4.2529047	-4.2258964	1.2365219

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	23.29	0.10653	YES	YES
8	a	35.24	0.53647	YES	YES
9	a	38.30	0.24444	YES	YES
10	a	41.19	0.96698	YES	YES
11	a	44.55	0.52232	YES	YES
12	a	48.02	0.54913	YES	YES
13	a	49.84	0.29528	YES	YES
14	a	59.13	0.39726	YES	YES
15	a	66.22	0.40964	YES	YES
16	a	86.93	0.62262	YES	YES
17	a	89.10	0.71655	YES	YES
18	a	103.42	0.07471	YES	YES
19	a	126.51	0.15680	YES	YES
20	a	130.66	0.25646	YES	YES
21	a	147.29	7.98522	YES	YES
22	a	172.29	10.05456	YES	YES
23	a	180.03	7.32537	YES	YES
24	a	210.81	4.81705	YES	YES
25	a	214.90	2.33947	YES	YES
26	a	245.05	2.54091	YES	YES
27	a	256.36	1.31831	YES	YES
28	a	296.20	2.60722	YES	YES
29	a	343.61	21.91165	YES	YES
30	a	369.80	7.55395	YES	YES
31	a	381.75	7.18937	YES	YES
32	a	399.35	0.30002	YES	YES
33	a	401.85	0.56329	YES	YES
34	a	402.76	0.87591	YES	YES
35	a	409.32	7.61748	YES	YES
36	a	428.58	6.12174	YES	YES
37	a	443.00	0.49891	YES	YES
38	a	466.45	8.99863	YES	YES
39	a	473.38	2.05015	YES	YES
40	a	486.00	0.75574	YES	YES
41	a	488.36	1.35608	YES	YES
42	a	503.69	5.89648	YES	YES
43	a	515.51	29.07783	YES	YES
44	a	522.48	28.37979	YES	YES
45	a	544.90	4.36957	YES	YES
46	a	555.70	32.56046	YES	YES
47	a	563.22	1.88397	YES	YES
48	a	594.11	46.25290	YES	YES
49	a	608.59	1.40299	YES	YES
50	a	610.70	4.43086	YES	YES

TS_{23aa}

SCF Energy (au) BP86/SV(P) -2427.864609133
SCF Energy (au) PBE0/def2-TZVPP -2427.423479953
SCF Energy (au) PBE0/def2-TZVPP -2427.4336311029 (Toluene Correction)
Zero Point Energy (au) 0.2961349
Chemical Potential (kJ mol^{-1}) 626.52
Dispersion Correction (au) PBE0/def2-TZVPP -0.06311849

xyz coordinates
43

Mn	1.6788083	0.5413038	0.6660746
C	2.0503776	0.5296482	2.4309562
C	3.4045443	0.1742659	0.2830201
C	2.0529433	2.3065225	0.5143330
O	2.3294949	3.4417091	0.4733818
O	4.5278610	0.0167896	0.0295371
O	2.2814247	0.4988557	3.5712309
C	-1.0926686	-0.2583324	1.3776519
C	-0.9973400	2.0490016	0.9698394
C	-2.3651450	2.2050745	1.2189961
C	-3.1234895	1.0695381	1.5546272
C	-2.4812563	-0.1687169	1.6297222
C	-0.3111906	-1.4899509	1.4194569
C	1.0201526	-1.3705871	0.9948310
C	1.8629472	-2.5728500	1.0052334
O	1.2773948	-3.7544008	1.5323100
C	-0.0161149	-3.8397296	1.9367080
C	-0.8418725	-2.7488364	1.8724334
O	2.9976265	-2.6790794	0.5829983
C	-0.3753289	-5.2043941	2.4389469
N	-0.3659046	0.8571799	1.0459106
C	0.3346785	1.3859714	-2.3672480
C	0.7595590	2.7269160	-2.5583839
C	0.2076688	3.5125802	-3.5802728
C	-0.7871582	2.9913869	-4.4262850
C	-1.2257909	1.6668207	-4.2433593
C	-0.6763379	0.8725536	-3.2295837
C	0.8900099	0.5081948	-1.3681614
C	1.2206952	-0.6756461	-0.9953258
H	-0.3749161	2.9150525	0.6987359
H	-2.8212774	3.2044537	1.1470848
H	-4.2045597	1.1511865	1.7526742
H	-3.0496886	-1.0765220	1.8787698
H	-1.8814572	-2.8487494	2.2152355
H	1.5379814	3.1497117	-1.9072265
H	0.5606496	4.5483909	-3.7161426
H	-1.2210490	3.6149772	-5.2253032
H	-2.0054478	1.2462192	-4.9007374
H	-1.0214133	-0.1641280	-3.0867825
H	1.6181458	-1.6329900	-1.3457148
H	-1.4359054	-5.2432596	2.7599516
H	0.2713780	-5.4850809	3.3010068
H	-0.2090293	-5.9710504	1.6488693

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-172.74	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-

6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	17.15	0.19902	YES	YES
9	a	25.26	0.83606	YES	YES
10	a	36.60	0.25361	YES	YES
11	a	50.78	1.18797	YES	YES
12	a	68.90	0.33269	YES	YES
13	a	75.37	0.27528	YES	YES
14	a	83.79	0.33993	YES	YES
15	a	86.74	0.04327	YES	YES
16	a	96.62	0.57822	YES	YES
17	a	109.43	0.42627	YES	YES
18	a	114.10	0.77591	YES	YES
19	a	125.09	0.29870	YES	YES
20	a	139.91	0.23751	YES	YES
21	a	147.81	0.17597	YES	YES
22	a	157.72	0.40932	YES	YES
23	a	160.75	0.93429	YES	YES
24	a	166.63	0.17092	YES	YES
25	a	197.22	0.23595	YES	YES
26	a	218.08	0.19371	YES	YES
27	a	240.38	0.46477	YES	YES
28	a	253.84	0.64059	YES	YES
29	a	263.01	0.61563	YES	YES
30	a	296.72	2.08692	YES	YES
31	a	326.39	1.40105	YES	YES
32	a	358.07	7.40260	YES	YES
33	a	400.87	3.17185	YES	YES
34	a	401.88	0.60941	YES	YES
35	a	413.51	2.56676	YES	YES
36	a	428.75	2.81648	YES	YES
37	a	445.21	21.76269	YES	YES
38	a	452.26	1.83643	YES	YES
39	a	464.49	7.14943	YES	YES
40	a	476.70	0.11278	YES	YES
41	a	488.43	2.37409	YES	YES
42	a	500.20	9.44866	YES	YES
43	a	518.27	3.03466	YES	YES
44	a	529.63	23.82817	YES	YES
45	a	541.63	1.06373	YES	YES
46	a	544.47	13.48474	YES	YES
47	a	549.76	9.80746	YES	YES
48	a	557.70	1.89472	YES	YES
49	a	578.36	4.12900	YES	YES
50	a	595.17	0.22690	YES	YES

TS_{23aa}'

SCF Energy (au) BP86/SV(P) -2427.853649810
SCF Energy (au) PBE0/def2-TZVPP -2427.411853990
SCF Energy (au) PBE0/def2-TZVPP -2427.4224059121 (Toluene Correction)
Zero Point Energy (au) 0.2956693
Chemical Potential (kJ mol^{-1}) 626.31
Dispersion Correction (au) PBE0/def2-TZVPP -0.06517125

xyz coordinates
43

Mn	1.0604984	1.9929986	0.6823022
C	1.1926923	1.9710117	2.4887800
C	2.8402352	1.7610039	0.5308806
C	1.3031491	3.7726719	0.5343487
O	1.4575616	4.9226638	0.4009624
O	3.9979345	1.6996050	0.4251379
O	1.2638844	1.9542238	3.6513366
C	-1.7427753	0.9781922	0.9238369
C	-1.7520834	3.3143000	0.7426142
C	-3.1498270	3.3684228	0.7892244
C	-3.8676255	2.1628212	0.8860943
C	-3.1576459	0.9614400	0.9491014
C	-0.8901215	-0.2022918	1.0187510
C	0.4721886	0.0135517	0.7444250
C	1.4114444	-1.0994791	0.9731314
O	0.8391756	-2.3394707	1.3652037
C	-0.4883289	-2.5283980	1.5730719
C	-1.3770827	-1.4975889	1.4105772
O	2.6192985	-1.0748372	0.8711519
C	-0.8132012	-3.9270560	1.9988310
N	-1.0561467	2.1591024	0.8084151
H	0.5555830	2.6948941	-2.1509651
C	0.6288065	1.9886473	-1.3183179
C	0.7477162	0.7162106	-1.1093196
H	-1.1579647	4.2371139	0.6524449
H	-3.6603325	4.3429790	0.7462084
H	-4.9694859	2.1626073	0.9105492
H	-3.6911847	0.0015311	1.0122905
H	-2.4402450	-1.6718158	1.6303188
C	1.1039835	-0.5017176	-1.8602694
H	-1.9022736	-4.0486906	2.1688486
H	-0.2713592	-4.1858413	2.9365708
H	-0.4852060	-4.6580329	1.2257502
C	1.7790484	-2.7511502	-3.4308975
C	0.5012548	-2.6531301	-2.8533448
C	0.1673545	-1.5412404	-2.0635187
C	2.3883301	-0.6098079	-2.4425055
C	2.7209197	-1.7283106	-3.2208056
H	2.0437175	-3.6285309	-4.0436556
H	-0.2420134	-3.4504317	-3.0172470
H	-0.8337747	-1.4639422	-1.6100762
H	3.1263228	0.1883341	-2.2657896
H	3.7275781	-1.8025624	-3.6644467

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-288.74	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-

6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	21.46	0.39886	YES	YES
9	a	30.55	0.36529	YES	YES
10	a	45.61	0.14736	YES	YES
11	a	48.26	1.22449	YES	YES
12	a	61.67	1.09460	YES	YES
13	a	78.38	0.44833	YES	YES
14	a	80.46	0.36741	YES	YES
15	a	86.87	0.15774	YES	YES
16	a	87.52	0.03196	YES	YES
17	a	102.02	0.56412	YES	YES
18	a	117.64	0.72443	YES	YES
19	a	128.81	0.28060	YES	YES
20	a	139.44	0.17071	YES	YES
21	a	151.48	0.37273	YES	YES
22	a	154.69	1.64005	YES	YES
23	a	163.17	0.10362	YES	YES
24	a	183.63	4.33893	YES	YES
25	a	193.95	0.97564	YES	YES
26	a	205.28	1.95662	YES	YES
27	a	217.80	0.71034	YES	YES
28	a	241.30	0.10665	YES	YES
29	a	260.18	0.11090	YES	YES
30	a	294.13	2.09385	YES	YES
31	a	318.15	4.59114	YES	YES
32	a	336.13	5.10675	YES	YES
33	a	393.18	3.92944	YES	YES
34	a	401.13	0.22347	YES	YES
35	a	424.46	2.13993	YES	YES
36	a	442.37	0.36676	YES	YES
37	a	455.80	1.51566	YES	YES
38	a	461.35	3.17289	YES	YES
39	a	478.45	0.81725	YES	YES
40	a	486.10	4.10302	YES	YES
41	a	497.65	8.36675	YES	YES
42	a	504.82	14.06983	YES	YES
43	a	519.59	6.15730	YES	YES
44	a	527.76	18.80972	YES	YES
45	a	539.96	1.42932	YES	YES
46	a	550.42	22.84540	YES	YES
47	a	556.16	4.99382	YES	YES
48	a	559.43	1.35728	YES	YES
49	a	577.03	5.35828	YES	YES
50	a	595.77	4.13113	YES	YES

TS_{23ba}

SCF Energy (au) BP86/SV(P) -2277.508412844
SCF Energy (au) PBE0/def2-TZVPP -2277.059214716
SCF Energy (au) PBE0/def2-TZVPP -2277.0663116709 (Toluene Correction)
Zero Point Energy (au) 0.2893905
Chemical Potential (kJ mol^{-1}) 617.01
Dispersion Correction (au) PBE0/def2-TZVPP -0.06065985

xyz coordinates
41

Mn	1.5462735	0.3705217	0.7753154
C	1.9074785	0.6310002	2.5277213
C	3.2407096	-0.1119005	0.4629426
C	1.9480722	2.0777093	0.3447596
O	2.2410160	3.1806368	0.0936545
O	4.3448104	-0.4362008	0.2648014
O	2.1292592	0.7906648	3.6591366
C	-1.2537830	-0.2555350	1.5959263
C	-1.0996745	1.9697746	0.8633464
C	-2.4649227	2.1924425	1.0617323
C	-3.2557673	1.1294770	1.5353928
C	-2.6464858	-0.0988281	1.7968796
C	-0.5014315	-1.4808271	1.8581717
C	0.8516553	-1.5011387	1.3910424
C	1.6375491	-2.6423727	1.7084079
C	1.1063609	-3.7167233	2.4268538
C	-0.2425309	-3.7004240	2.8496778
C	-1.0364875	-2.5874485	2.5642042
H	-0.4503635	2.7714576	0.4801914
H	-2.8950271	3.1812287	0.8405819
H	-4.3388895	1.2594921	1.6936461
H	-3.2441232	-0.9503939	2.1538562
H	2.6862936	-2.6887826	1.3693071
H	1.7476473	-4.5817195	2.6667466
H	-0.6612248	-4.5507498	3.4116467
H	-2.0786672	-2.5634039	2.9225327
N	-0.5004788	0.7858067	1.1211501
C	0.3494049	0.6612376	-2.3782613
C	0.9745764	1.8354334	-2.8740594
C	0.5652123	2.4058176	-4.0878125
C	-0.4881425	1.8378149	-4.8263467
C	-1.1277044	0.6820037	-4.3411795
C	-0.7159981	0.0978621	-3.1365469
H	1.7966554	2.2946711	-2.3060925
H	1.0739469	3.3109476	-4.4593641
H	-0.8125999	2.2955425	-5.7753977
H	-1.9568402	0.2282210	-4.9096864
H	-1.2183045	-0.8065564	-2.7569113
C	0.7583943	0.0048373	-1.1586284
C	0.9391618	-1.1406739	-0.5838789
H	1.1481747	-2.1808689	-0.8504819

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-230.16	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-

8	a	15.33	0.05488	YES	YES
9	a	25.28	0.19576	YES	YES
10	a	45.61	0.05019	YES	YES
11	a	58.66	0.11086	YES	YES
12	a	71.59	0.08026	YES	YES
13	a	82.53	0.01510	YES	YES
14	a	89.55	0.28337	YES	YES
15	a	92.92	1.09647	YES	YES
16	a	100.46	0.46379	YES	YES
17	a	109.98	0.06435	YES	YES
18	a	116.38	0.03637	YES	YES
19	a	132.51	0.35585	YES	YES
20	a	162.15	1.17092	YES	YES
21	a	182.00	0.54087	YES	YES
22	a	187.25	0.55331	YES	YES
23	a	217.10	0.99499	YES	YES
24	a	233.54	0.82810	YES	YES
25	a	259.73	0.63802	YES	YES
26	a	278.83	0.12353	YES	YES
27	a	343.57	8.45214	YES	YES
28	a	359.38	1.36759	YES	YES
29	a	385.36	2.37851	YES	YES
30	a	402.36	0.07350	YES	YES
31	a	415.74	3.16983	YES	YES
32	a	430.74	1.25286	YES	YES
33	a	447.29	0.41322	YES	YES
34	a	453.95	8.13841	YES	YES
35	a	463.51	5.86149	YES	YES
36	a	474.07	1.00384	YES	YES
37	a	488.83	0.36260	YES	YES
38	a	496.72	7.61252	YES	YES
39	a	503.64	5.23803	YES	YES
40	a	522.87	0.37797	YES	YES
41	a	544.04	13.92394	YES	YES
42	a	546.27	13.93147	YES	YES
43	a	553.19	0.61857	YES	YES
44	a	583.04	24.49030	YES	YES
45	a	610.29	10.92190	YES	YES
46	a	614.19	12.97094	YES	YES
47	a	620.33	1.05024	YES	YES
48	a	625.80	33.87210	YES	YES
49	a	639.10	0.33601	YES	YES
50	a	656.26	9.87788	YES	YES

TS_{23ba}'

SCF Energy (au) BP86/SV(P) -2277.498753669
SCF Energy (au) PBE0/def2-TZVPP -2277.050675757
SCF Energy (au) PBE0/def2-TZVPP -2277.0579338980 (Toluene Correction)
Zero Point Energy (au) 0.2891519
Chemical Potential (kJ mol^{-1}) 617.56
Dispersion Correction (au) PBE0/def2-TZVPP -0.06291758

xyz coordinates
41

Mn	1.1693515	1.7942172	0.3501382
C	1.3530807	2.1824100	2.1120978
C	2.8984100	1.3543494	0.2491536
C	1.5418946	3.4606063	-0.2139974
O	1.7908638	4.5248368	-0.6268932
O	4.0275882	1.0587937	0.1914371
O	1.4670734	2.4424552	3.2421069
C	-1.6743451	1.0921558	0.9437799
C	-1.5381688	3.2923065	0.1440870
C	-2.9237216	3.4672754	0.2150309
C	-3.7137545	2.3901122	0.6558466
C	-3.0839075	1.1971132	1.0167486
C	-0.9017448	-0.0900528	1.3304482
C	0.4690251	-0.1133275	0.9201197
C	1.2675083	-1.2000501	1.3628840
C	0.7451521	-2.2018261	2.1868477
C	-0.6142475	-2.1778035	2.5683531
C	-1.4316588	-1.1289586	2.1356710
H	-0.8861808	4.1064682	-0.2083692
H	-3.3692387	4.4305340	-0.0775210
H	-4.8108328	2.4810647	0.7124324
H	-3.6776879	0.3328533	1.3496471
H	2.3232634	-1.2577098	1.0512727
H	1.4009614	-3.0169031	2.5362660
H	-1.0266261	-2.9709426	3.2128557
H	-2.4836241	-1.0931220	2.4637971
N	-0.9209399	2.1431123	0.4957934
H	0.6382497	1.8377141	-2.5520672
C	0.6896772	1.3458523	-1.5751871
C	0.6556402	0.1490567	-1.0778296
C	0.8042723	-1.2237752	-1.5915096
C	1.0787431	-3.7779246	-2.7828737
C	2.0089812	-2.7639563	-3.0681654
C	1.8725870	-1.4960946	-2.4811888
C	-0.1193572	-2.2559564	-1.3035661
C	0.0135775	-3.5173396	-1.9016755
H	1.1842179	-4.7734357	-3.2452973
H	2.8502730	-2.9600918	-3.7535367
H	2.6014809	-0.6992120	-2.6983808
H	-0.9532646	-2.0579155	-0.6121681
H	-0.7225716	-4.3068894	-1.6765880

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-281.20	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-

8	a	24.93	0.17999	YES	YES
9	a	27.66	0.48622	YES	YES
10	a	45.67	0.02077	YES	YES
11	a	62.41	0.22472	YES	YES
12	a	65.71	0.29527	YES	YES
13	a	78.12	0.03628	YES	YES
14	a	88.38	0.19623	YES	YES
15	a	91.74	0.15481	YES	YES
16	a	100.11	0.55229	YES	YES
17	a	104.64	0.31790	YES	YES
18	a	117.99	0.09532	YES	YES
19	a	140.73	0.44197	YES	YES
20	a	163.87	0.86445	YES	YES
21	a	173.92	2.70349	YES	YES
22	a	194.82	1.83630	YES	YES
23	a	215.19	2.41823	YES	YES
24	a	221.11	2.12687	YES	YES
25	a	248.39	0.85224	YES	YES
26	a	282.00	0.34236	YES	YES
27	a	311.11	3.32284	YES	YES
28	a	357.00	1.24876	YES	YES
29	a	402.97	0.19811	YES	YES
30	a	405.95	4.72270	YES	YES
31	a	412.17	4.75989	YES	YES
32	a	438.81	1.52677	YES	YES
33	a	459.78	0.38930	YES	YES
34	a	464.82	0.37031	YES	YES
35	a	476.22	0.84671	YES	YES
36	a	488.03	1.90597	YES	YES
37	a	495.73	1.86045	YES	YES
38	a	503.95	1.64839	YES	YES
39	a	508.14	20.16433	YES	YES
40	a	530.44	4.19986	YES	YES
41	a	536.50	13.61825	YES	YES
42	a	551.86	3.52941	YES	YES
43	a	558.62	18.82493	YES	YES
44	a	563.39	4.96911	YES	YES
45	a	607.86	39.79700	YES	YES
46	a	613.27	0.66942	YES	YES
47	a	619.75	1.86931	YES	YES
48	a	625.45	41.97016	YES	YES
49	a	639.98	3.75850	YES	YES
50	a	655.90	36.17631	YES	YES

TS_{23bb}

SCF Energy (au) BP86/SV(P) -2505.228414752
SCF Energy (au) PBE0/def2-TZVPP -2504.778820226
SCF Energy (au) PBE0/def2-TZVPP -2504.7885430275 (Toluene Correction)
Zero Point Energy (au) 0.3313323
Chemical Potential (kJ mol^{-1}) 705.79
Dispersion Correction (au) PBE0/def2-TZVPP -0.06493997

xyz coordinates
47

Mn	1.5438696	0.9121769	1.8459137
C	2.0798231	0.9719827	3.5736955
C	3.1974123	0.4569030	1.3335957
C	1.9102005	2.6474432	1.5317027
O	2.1536748	3.7650521	1.2941777
O	4.2787058	0.1493930	1.0206017
O	2.4160219	1.0083613	4.6878982
C	-1.1654630	0.1794923	2.8715540
C	-1.0519913	2.4881328	2.4653612
C	-2.3845969	2.6819223	2.8412507
C	-3.1387447	1.5606537	3.2329710
C	-2.5251532	0.3067525	3.2449353
C	-0.4090617	-1.0728962	2.8813346
C	0.8736495	-1.0406434	2.2486695
C	1.6714458	-2.2132932	2.3163424
C	1.2170098	-3.3654072	2.9657126
C	-0.0642883	-3.3954557	3.5605320
C	-0.8684506	-2.2533241	3.5161742
H	-0.4291977	3.3392628	2.1480412
H	-2.8179453	3.6938075	2.8222620
H	-4.1964514	1.6664260	3.5247371
H	-3.0947039	-0.5874665	3.5376316
H	2.6647491	-2.2217370	1.8373571
H	1.8666377	-4.2555965	3.0141119
H	-0.4225746	-4.3057289	4.0675956
H	-1.8534569	-2.2681725	4.0106361
N	-0.4512635	1.2776419	2.4717770
C	0.3693367	1.7188046	-1.1444068
C	0.6498899	0.8052351	-0.0221054
C	0.7090328	-0.4233841	0.3630955
H	0.6788933	-1.4385500	-0.0426014
O	-0.1688441	1.0330044	-2.3015015
H	-0.4003790	2.4718013	-0.8668055
H	1.2983409	2.2526720	-1.4426764
C	0.7049208	0.7742823	-3.3204458
O	1.8753878	1.1155984	-3.3111180
C	0.0472152	0.0363104	-4.4440085
C	-1.0840302	-1.3458045	-6.6194205
C	-1.8713107	-1.0393509	-5.4947766
C	-1.3103816	-0.3504427	-4.4085130
C	0.8333988	-0.2740593	-5.5746196
C	0.2691938	-0.9621104	-6.6578499
H	-1.5277977	-1.8874805	-7.4714750
H	-2.9315905	-1.3404367	-5.4649314
H	-1.9178860	-0.1074050	-3.5239907
H	1.8897097	0.0374432	-5.5794971
H	0.8870432	-1.2018104	-7.5389247

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
#					
1	a	-244.44	0.00000	YES	YES

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	10.09	0.14991	YES	YES
9	a	12.41	0.42334	YES	YES
10	a	19.22	0.07028	YES	YES
11	a	36.42	0.34341	YES	YES
12	a	49.37	0.00449	YES	YES
13	a	53.56	1.03068	YES	YES
14	a	63.81	0.10861	YES	YES
15	a	68.11	0.21311	YES	YES
16	a	81.72	0.07782	YES	YES
17	a	91.80	0.56193	YES	YES
18	a	94.63	0.43159	YES	YES
19	a	101.38	0.53503	YES	YES
20	a	106.77	0.28635	YES	YES
21	a	122.46	0.47390	YES	YES
22	a	144.26	0.30543	YES	YES
23	a	165.36	0.72460	YES	YES
24	a	171.49	0.24320	YES	YES
25	a	185.89	0.55184	YES	YES
26	a	213.01	0.47639	YES	YES
27	a	230.75	3.89429	YES	YES
28	a	239.47	1.28996	YES	YES
29	a	248.79	3.55678	YES	YES
30	a	275.42	0.73147	YES	YES
31	a	280.32	1.12081	YES	YES
32	a	328.93	26.14672	YES	YES
33	a	358.46	1.92623	YES	YES
34	a	362.92	3.07572	YES	YES
35	a	404.07	0.86355	YES	YES
36	a	404.41	2.01337	YES	YES
37	a	417.15	1.67101	YES	YES
38	a	431.57	5.04544	YES	YES
39	a	439.66	0.34171	YES	YES
40	a	446.69	1.08182	YES	YES
41	a	461.13	0.75367	YES	YES
42	a	471.59	3.36562	YES	YES
43	a	483.05	4.85382	YES	YES
44	a	487.66	0.99726	YES	YES
45	a	495.49	1.19401	YES	YES
46	a	503.25	1.96319	YES	YES
47	a	538.01	10.91463	YES	YES
48	a	541.54	18.16062	YES	YES
49	a	555.44	1.04452	YES	YES
50	a	608.16	29.89436	YES	YES

TS_{23bb}'

SCF Energy (au) BP86/SV(P) -2505.224054475
SCF Energy (au) PBE0/def2-TZVPP -2504.774662695
SCF Energy (au) PBE0/def2-TZVPP -2504.7841905779 (Toluene Correction)
Zero Point Energy (au) 0.3314439
Chemical Potential (kJ mol^{-1}) 709.37
Dispersion Correction (au) PBE0/def2-TZVPP -0.06628063

xyz coordinates
47

Mn	1.2176947	1.8127312	1.4456319
C	1.4666299	2.4182820	3.1346110
C	2.8893178	1.1728893	1.4137244
C	1.7679512	3.3323829	0.6551328
O	2.1268865	4.2962021	0.1018704
O	3.9807488	0.7592320	1.4167611
O	1.6187517	2.8163816	4.2189751
C	-1.6838173	1.5142621	2.1055525
C	-1.2983862	3.5883820	1.0814943
C	-2.6544880	3.9279053	1.1212621
C	-3.5615029	3.0007085	1.6654012
C	-3.0715137	1.7883817	2.1557660
C	-1.0522446	0.3000024	2.6278138
C	0.3178775	0.0931789	2.2594279
C	0.9900761	-1.0164614	2.8399414
C	0.3403405	-1.8804578	3.7303729
C	-1.0174117	-1.6817832	4.0587049
C	-1.7050384	-0.5940762	3.5088041
H	-0.5586526	4.2812524	0.6514182
H	-2.9875741	4.8995658	0.7252030
H	-4.6407100	3.2219184	1.7026697
H	-3.7603152	1.0398129	2.5746974
H	2.0494275	-1.1997610	2.5938167
H	0.8985435	-2.7185790	4.1805668
H	-1.5292451	-2.3650339	4.7553365
H	-2.7527021	-0.4154062	3.8017342
N	-0.8163498	2.4183728	1.5543468
H	0.6856472	1.5157013	-1.4528148
C	0.6638975	1.1671894	-0.4166241
C	0.4808754	0.0959589	0.2799620
C	0.2934903	-1.3751688	0.0287064
H	1.1764943	-1.9454385	0.3875599
O	0.1108113	-1.6183489	-1.3743703
H	-0.6198903	-1.7588766	0.5291987
C	1.2148822	-2.0214416	-2.0778786
C	0.9116156	-2.2027878	-3.5308409
O	2.3038448	-2.2167652	-1.5675274
C	0.4570424	-2.5830452	-6.2818126
C	-0.5934419	-2.1600732	-5.4474376
C	-0.3701491	-1.9689868	-4.0754074
C	1.9629695	-2.6268606	-4.3723148
C	1.7357560	-2.8156257	-5.7425261
H	0.2779652	-2.7320770	-7.3598355
H	-1.5950647	-1.9776276	-5.8706516
H	-1.1845808	-1.6372763	-3.4145553
H	2.9540616	-2.8025317	-3.9254058
H	2.5594795	-3.1462033	-6.3964612

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-278.19	0.00000	YES	YES

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	14.29	0.20383	YES	YES
9	a	18.08	0.34253	YES	YES
10	a	22.29	0.24399	YES	YES
11	a	44.01	0.53700	YES	YES
12	a	48.83	0.03663	YES	YES
13	a	55.33	0.76764	YES	YES
14	a	62.75	0.67513	YES	YES
15	a	72.87	0.20665	YES	YES
16	a	81.93	0.03362	YES	YES
17	a	91.19	0.30181	YES	YES
18	a	97.97	0.10896	YES	YES
19	a	100.80	0.65510	YES	YES
20	a	104.64	0.37368	YES	YES
21	a	131.83	0.49765	YES	YES
22	a	143.99	0.40575	YES	YES
23	a	153.64	0.20252	YES	YES
24	a	174.60	0.14773	YES	YES
25	a	189.03	0.20652	YES	YES
26	a	212.84	2.82187	YES	YES
27	a	221.80	0.80722	YES	YES
28	a	240.53	0.72260	YES	YES
29	a	261.29	0.28153	YES	YES
30	a	281.46	0.06689	YES	YES
31	a	337.95	16.67654	YES	YES
32	a	345.86	3.26526	YES	YES
33	a	370.77	4.72862	YES	YES
34	a	372.63	8.71314	YES	YES
35	a	404.28	0.00737	YES	YES
36	a	416.30	4.57346	YES	YES
37	a	428.03	2.77797	YES	YES
38	a	438.60	0.63452	YES	YES
39	a	447.54	4.17340	YES	YES
40	a	457.06	1.37976	YES	YES
41	a	464.31	0.81569	YES	YES
42	a	474.49	7.60730	YES	YES
43	a	486.49	5.48000	YES	YES
44	a	492.07	3.12404	YES	YES
45	a	497.16	0.53026	YES	YES
46	a	520.26	8.99771	YES	YES
47	a	536.66	8.13746	YES	YES
48	a	539.91	7.75461	YES	YES
49	a	557.69	1.52783	YES	YES
50	a	594.61	14.24688	YES	YES

TS_{23bc}

SCF Energy (au) BP86/SV(P) -2281.108277972
SCF Energy (au) PBE0/def2-TZVPP -2280.675226907
SCF Energy (au) PBE0/def2-TZVPP -2280.6812177349 (Toluene Correction)
Zero Point Energy (au) 0.3569715
Chemical Potential (kJ mol^{-1}) 792.89
Dispersion Correction (au) PBE0/def2-TZVPP -0.06589746

xyz coordinates
47

Mn	1.2409727	0.0904313	1.1054278
C	1.7311248	0.3069725	2.8341453
C	2.9349362	-0.2493845	0.6484351
C	1.4660984	1.8319250	0.7125130
O	1.6364875	2.9606134	0.4571049
O	4.0432610	-0.4834398	0.3624492
O	2.0488129	0.4436701	3.9464924
C	-1.4110895	-0.8149669	2.1472777
C	-1.4941407	1.4652372	1.6033007
C	-2.8401766	1.5663616	1.9674951
C	-3.4994615	0.4091231	2.4211488
C	-2.7800988	-0.7837775	2.5083186
C	-0.5475761	-1.9909043	2.2519126
C	0.7415510	-1.8796712	1.6418711
C	1.6444047	-2.9638656	1.8098994
C	1.2824482	-4.1071377	2.5287496
C	-0.0064634	-4.2200319	3.0972038
C	-0.9113734	-3.1642600	2.9579791
H	-0.9461394	2.3464649	1.2361120
H	-3.3574921	2.5350863	1.8893364
H	-4.5644064	0.4401332	2.7038761
H	-3.2718994	-1.7047943	2.8544300
H	2.6470104	-2.9102543	1.3538155
H	2.0115115	-4.9257753	2.6532134
H	-0.2919077	-5.1243727	3.6582021
H	-1.9036072	-3.2389523	3.4322280
N	-0.7912019	0.3135281	1.6784625
C	0.2036167	0.4229103	-2.1177340
C	0.4513932	-0.2496748	-0.8076748
C	0.5544724	-1.4233179	-0.2809152
H	0.5633337	-2.4760312	-0.5790808
C	1.5251228	0.9180035	-2.7641032
H	-0.2221469	-0.3552697	-2.7995672
C	-0.8249443	1.5785412	-2.0498146
H	1.9931170	1.6754389	-2.0945966
C	1.2743359	1.5382902	-4.1498764
H	2.2434790	0.0717299	-2.8390196
C	-1.0745684	2.1931968	-3.4382736
H	-0.4370484	2.3638521	-1.3613850
H	-1.7785201	1.2070255	-1.6127079
H	2.2338584	1.9152600	-4.5702918
C	0.2347654	2.6710113	-4.0898355
H	0.9156396	0.7455923	-4.8492349
H	-1.7966169	3.0368433	-3.3533072
H	-1.5580063	1.4319299	-4.0963259
H	0.0361840	3.0674924	-5.1113184
H	0.6509482	3.5192177	-3.4963377

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-233.32	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	25.44	0.27019	YES	YES
9	a	35.20	0.13176	YES	YES
10	a	46.20	0.02342	YES	YES
11	a	53.63	0.13003	YES	YES
12	a	66.66	0.05869	YES	YES
13	a	78.23	0.40040	YES	YES
14	a	89.32	0.15455	YES	YES
15	a	92.83	0.72234	YES	YES
16	a	100.02	0.31098	YES	YES
17	a	107.64	0.22848	YES	YES
18	a	111.47	0.08287	YES	YES
19	a	118.84	0.19875	YES	YES
20	a	139.08	0.70360	YES	YES
21	a	164.03	0.45277	YES	YES
22	a	178.62	0.17963	YES	YES
23	a	203.50	0.48532	YES	YES
24	a	222.28	0.01933	YES	YES
25	a	230.18	2.70261	YES	YES
26	a	252.56	0.24883	YES	YES
27	a	275.88	0.27280	YES	YES
28	a	297.12	0.59696	YES	YES
29	a	350.68	0.94622	YES	YES
30	a	357.11	3.26921	YES	YES
31	a	369.95	2.21091	YES	YES
32	a	406.80	5.59754	YES	YES
33	a	420.17	1.06675	YES	YES
34	a	426.52	2.17763	YES	YES
35	a	438.74	0.84404	YES	YES
36	a	454.19	11.41550	YES	YES
37	a	459.39	1.23093	YES	YES
38	a	471.27	2.01419	YES	YES
39	a	471.95	3.22404	YES	YES
40	a	489.54	1.07058	YES	YES
41	a	497.71	3.64178	YES	YES
42	a	501.29	0.55328	YES	YES
43	a	512.85	3.57526	YES	YES
44	a	538.43	8.95694	YES	YES
45	a	546.38	13.34263	YES	YES
46	a	554.60	0.78629	YES	YES
47	a	575.01	5.02399	YES	YES
48	a	608.92	30.54046	YES	YES
49	a	620.85	1.38396	YES	YES
50	a	626.27	27.58342	YES	YES

TS_{23bc}'

SCF Energy (au) BP86/SV(P) -2281.103977722
SCF Energy (au) PBE0/def2-TZVPP -2280.671218205
SCF Energy (au) PBE0/def2-TZVPP -2280.6773988784 (Toluene Correction)
Zero Point Energy (au) 0.3568424
Chemical Potential (kJ mol^{-1}) 797.65
Dispersion Correction (au) PBE0/def2-TZVPP -0.06661635

xyz coordinates
47

Mn	1.0584974	2.0075745	0.8636094
C	1.4065610	2.2963033	2.6176727
C	2.7788548	1.6425535	0.5573960
C	1.3205956	3.7147665	0.3651363
O	1.4974053	4.8097286	-0.0032252
O	3.9057319	1.3940366	0.3681308
O	1.6234799	2.4911867	3.7462495
C	-1.7061683	1.1522758	1.6243631
C	-1.6886102	3.4310935	1.0701333
C	-3.0684950	3.5500041	1.2626764
C	-3.7950418	2.4032639	1.6319445
C	-3.1089848	1.2000750	1.8086790
C	-0.8726400	-0.0319920	1.8388759
C	0.4736055	0.0450664	1.3512083
C	1.3479316	-1.0237779	1.6922311
C	0.9071021	-2.1236832	2.4369192
C	-0.4377380	-2.2114362	2.8578647
C	-1.3174290	-1.1648302	2.5617230
H	-1.0871356	4.3015186	0.7649208
H	-3.5595699	4.5246115	1.1173136
H	-4.8867356	2.4495819	1.7772479
H	-3.6530995	0.2847545	2.0850452
H	2.4021464	-0.9837975	1.3745237
H	1.6198810	-2.9228353	2.7019266
H	-0.7867523	-3.0815597	3.4369294
H	-2.3524705	-1.2085626	2.9388834
N	-1.0173060	2.2713703	1.2407304
H	0.2052153	2.1992758	-1.9447688
C	0.3697731	1.6399617	-1.0188688
C	0.4261576	0.4189076	-0.5900383
C	0.4748275	-0.9544359	-1.2231924
C	-0.5425282	-1.0274437	-2.3907468
H	0.1864101	-1.7265873	-0.4769103
C	1.8966294	-1.2981526	-1.7380544
C	1.9297454	-2.6760491	-2.4233278
H	2.6279615	-1.2662767	-0.9017107
H	2.2091946	-0.5067970	-2.4582144
H	-1.5643380	-0.8028396	-2.0120097
C	-0.5107904	-2.4069750	-3.0738193
H	-0.2949055	-0.2366847	-3.1362682
H	-0.8600705	-3.1820754	-2.3511143
H	-1.2319186	-2.4215374	-3.9225519
H	1.7134871	-3.4671955	-1.6670317
H	2.9551625	-2.8796649	-2.8066906
C	0.9019421	-2.7681382	-3.5641145
H	0.9073472	-3.7886735	-4.0097542
H	1.1970819	-2.0659092	-4.3799218

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-292.01	0.00000	YES	YES
2	a	-3.78	0.00000	YES	YES
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8		0.00	0.00000	-	-
9	a	28.49	0.43330	YES	YES
10	a	46.44	0.00067	YES	YES
11	a	51.71	0.11284	YES	YES
12	a	64.85	0.27708	YES	YES
13	a	79.34	0.02072	YES	YES
14	a	89.33	0.29511	YES	YES
15	a	92.02	0.20021	YES	YES
16	a	101.05	0.72661	YES	YES
17	a	104.97	0.29552	YES	YES
18	a	111.48	0.11726	YES	YES
19	a	127.74	0.14195	YES	YES
20	a	163.52	1.93071	YES	YES
21	a	168.19	0.28006	YES	YES
22	a	171.57	0.06476	YES	YES
23	a	201.66	2.28831	YES	YES
24	a	221.68	0.90382	YES	YES
25	a	228.11	0.13987	YES	YES
26	a	240.12	0.50932	YES	YES
27	a	263.48	0.36210	YES	YES
28	a	281.08	0.10385	YES	YES
29	a	342.96	0.25244	YES	YES
30	a	356.62	1.72735	YES	YES
31	a	407.65	3.82895	YES	YES
32	a	413.53	1.94417	YES	YES
33	a	420.48	4.32053	YES	YES
34	a	430.59	1.93295	YES	YES
35	a	441.75	1.74368	YES	YES
36	a	460.81	2.24741	YES	YES
37	a	463.86	0.83593	YES	YES
38	a	483.58	1.45069	YES	YES
39	a	486.62	1.58686	YES	YES
40	a	495.34	0.90332	YES	YES
41	a	501.19	0.27970	YES	YES
42	a	520.05	2.89286	YES	YES
43	a	523.61	6.81593	YES	YES
44	a	539.03	12.66528	YES	YES
45	a	548.96	4.06695	YES	YES
46	a	559.92	3.76532	YES	YES
47	a	587.65	7.96722	YES	YES
48	a	609.87	30.76435	YES	YES
49	a	621.24	4.29310	YES	YES
50	a	627.98	39.61848	YES	YES

TS_{23bd}

SCF Energy (au) BP86/SV(P) -2411.377999102
SCF Energy (au) PBE0/def2-TZVPP -2410.917172120
SCF Energy (au) PBE0/def2-TZVPP -2410.9254826611 (Toluene Correction)
Zero Point Energy (au) 0.3599214
Chemical Potential (kJ mol^{-1}) 787.62
Dispersion Correction (au) PBE0/def2-TZVPP -0.06897874

xyz coordinates

49			
Mn	1.6834630	-0.0525723	1.9499502
C	2.0090554	0.2577901	3.6992573
C	3.3713646	-0.5845235	1.6926125
C	2.1363629	1.6313506	1.4813795
O	2.4693042	2.7221616	1.2212537
O	4.4707655	-0.9441518	1.5293227
O	2.2100084	0.4495467	4.8302512
C	-1.1470986	-0.5976926	2.7197754
C	-0.9324977	1.5925442	1.9007414
C	-2.2982368	1.8471218	2.0506641
C	-3.1213617	0.8185427	2.5459622
C	-2.5420504	-0.4077008	2.8750646
C	-0.4262491	-1.8243502	3.0472378
C	0.9386815	-1.8829973	2.6156958
C	1.6931261	-3.0281449	2.9933610
C	1.1210401	-4.0697105	3.7279511
C	-0.2386122	-4.0167145	4.1126819
C	-1.0019301	-2.8981569	3.7716426
H	-0.2574610	2.3661431	1.5045454
H	-2.7036819	2.8331761	1.7769299
H	-4.2059321	0.9735543	2.6683121
H	-3.1647403	-1.2331882	3.2502307
H	2.7509778	-3.1042007	2.6890843
H	1.7393524	-4.9380311	4.0129915
H	-0.6882753	-4.8412553	4.6890756
H	-2.0532278	-2.8431750	4.0993318
N	-0.3619388	0.4102460	2.2236019
C	0.5722182	0.1518922	-1.2459288
C	1.1001983	1.3866554	-1.7046310
C	0.7455663	1.9262172	-2.9429411
C	-0.1863450	1.2707796	-3.8004005
C	-0.7356187	0.0382648	-3.3340738
C	-0.3620324	-0.4981225	-2.1018884
H	1.8215642	1.9339246	-1.0809394
H	1.2023613	2.8797746	-3.2433579
N	-0.5456798	1.8075638	-5.0264299
H	-1.4654832	-0.5137298	-3.9434549
H	-0.8068323	-1.4520759	-1.7746075
C	0.9425459	-0.4725647	-0.0024645
C	1.0810974	-1.5992534	0.6214019
H	1.3031505	-2.6483348	0.4068866
C	-1.4962568	1.1107966	-5.8746984
C	0.0455147	3.0575437	-5.4719449
H	-0.1894395	3.9030832	-4.7811889
H	-0.3548213	3.3171793	-6.4718110
H	1.1569677	2.9896755	-5.5569684
H	-1.1337429	0.0962807	-6.1692087
H	-1.6569254	1.6947161	-6.8027670
H	-2.4882151	0.9841219	-5.3774916

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-232.90	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	17.63	0.42854	YES	YES
9	a	23.50	0.02888	YES	YES
10	a	39.27	0.17692	YES	YES
11	a	52.61	0.70633	YES	YES
12	a	60.93	0.75764	YES	YES
13	a	69.86	0.00642	YES	YES
14	a	73.50	0.05396	YES	YES
15	a	79.07	0.32040	YES	YES
16	a	87.05	0.20507	YES	YES
17	a	91.02	0.05740	YES	YES
18	a	93.52	1.26300	YES	YES
19	a	102.25	0.54171	YES	YES
20	a	109.71	0.09419	YES	YES
21	a	113.69	0.14201	YES	YES
22	a	133.88	0.09814	YES	YES
23	a	172.62	0.27658	YES	YES
24	a	173.33	0.33520	YES	YES
25	a	192.99	0.53918	YES	YES
26	a	203.92	0.52000	YES	YES
27	a	211.52	0.00193	YES	YES
28	a	232.77	1.06116	YES	YES
29	a	249.78	0.59980	YES	YES
30	a	259.75	0.23298	YES	YES
31	a	279.20	0.33588	YES	YES
32	a	294.51	4.85642	YES	YES
33	a	341.09	0.32281	YES	YES
34	a	358.51	3.22369	YES	YES
35	a	396.61	1.95742	YES	YES
36	a	412.41	1.72339	YES	YES
37	a	419.20	0.32576	YES	YES
38	a	428.07	21.42381	YES	YES
39	a	434.00	1.48273	YES	YES
40	a	443.83	5.47313	YES	YES
41	a	459.17	0.37495	YES	YES
42	a	467.34	6.59154	YES	YES
43	a	473.89	0.79606	YES	YES
44	a	481.82	2.47340	YES	YES
45	a	494.42	3.20775	YES	YES
46	a	502.22	4.26468	YES	YES
47	a	507.05	10.25813	YES	YES
48	a	526.69	7.26318	YES	YES
49	a	543.84	16.93748	YES	YES
50	a	545.01	27.45832	YES	YES

TS_{23bd}'

SCF Energy (au) BP86/SV(P) -2411.368746066
SCF Energy (au) PBE0/def2-TZVPP -2410.909311614
SCF Energy (au) PBE0/def2-TZVPP -2410.9178265345 (Toluene Correction)
Zero Point Energy (au) 0.3597223
Chemical Potential (kJ mol^{-1}) 787.33
Dispersion Correction (au) PBE0/def2-TZVPP -0.07129753

xyz coordinates
49

Mn	0.8765013	2.7963850	0.9256197
C	0.9665915	3.2424892	2.6802605
C	2.6063238	2.3530971	0.9199746
C	1.2790913	4.4416824	0.3257752
O	1.5517344	5.4917965	-0.1099508
O	3.7367907	2.0547615	0.9224713
O	1.0198641	3.5439671	3.8052743
C	-1.9912887	2.1018574	1.3960254
C	-1.8177428	4.2754438	0.5328868
C	-3.2051678	4.4498593	0.5301760
C	-4.0151754	3.3853344	0.9656546
C	-3.4030226	2.2059291	1.3950251
C	-1.2377681	0.9352140	1.8589081
C	0.1509035	0.9026020	1.5138263
C	0.9280650	-0.1658238	2.0340893
C	0.3691824	-1.1376972	2.8695596
C	-1.0078131	-1.1055827	3.1834053
C	-1.8056209	-0.0770676	2.6726767
H	-1.1489615	5.0789482	0.1874558
H	-3.6362272	5.4026418	0.1861606
H	-5.1138208	3.4754524	0.9651434
H	-4.0118098	1.3510936	1.7253487
H	1.9974218	-0.2319363	1.7741643
H	1.0090422	-1.9362397	3.2817040
H	-1.4492273	-1.8762165	3.8362410
H	-2.8727223	-0.0335685	2.9468625
N	-1.2177181	3.1397826	0.9516331
H	0.4686035	2.7499073	-1.9910079
C	0.4881411	2.2803288	-1.0018763
C	0.4290407	1.0882186	-0.4932435
C	0.6288202	-0.2901795	-0.9466634
C	1.0131190	-2.9201236	-2.0568575
C	1.9062441	-1.8495803	-2.3563812
C	1.7108367	-0.5755514	-1.8163986
C	-0.2496384	-1.3560608	-0.6375642
C	-0.0745392	-2.6310950	-1.1787563
N	1.1945533	-4.1852326	-2.5914633
H	2.7696160	-2.0099100	-3.0174565
H	2.4214364	0.2297555	-2.0624777
H	-1.1022642	-1.1757743	0.0361319
H	-0.7974877	-3.4146339	-0.9115329
C	0.2833252	-5.2604066	-2.2400371
C	2.3290919	-4.4509679	-3.4588670
H	3.3052120	-4.2826688	-2.9419781
H	2.3149097	-3.8095463	-4.3723163
H	2.2986772	-5.5081616	-3.7892528
H	-0.7685960	-5.0289145	-2.5330402
H	0.2886267	-5.4784424	-1.1443368
H	0.5848459	-6.1851661	-2.7709959

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-281.14	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	20.19	0.87179	YES	YES
9	a	27.26	0.34281	YES	YES
10	a	38.91	0.12241	YES	YES
11	a	48.94	0.33750	YES	YES
12	a	62.05	0.55669	YES	YES
13	a	65.23	0.13583	YES	YES
14	a	73.20	0.38913	YES	YES
15	a	80.39	0.02581	YES	YES
16	a	83.34	0.07330	YES	YES
17	a	89.03	0.82535	YES	YES
18	a	98.01	0.35279	YES	YES
19	a	103.39	0.62865	YES	YES
20	a	103.76	0.08370	YES	YES
21	a	128.54	0.82791	YES	YES
22	a	136.25	0.50399	YES	YES
23	a	151.00	8.53754	YES	YES
24	a	172.53	1.79403	YES	YES
25	a	173.86	0.17583	YES	YES
26	a	205.54	2.72256	YES	YES
27	a	208.09	0.60019	YES	YES
28	a	220.35	1.63172	YES	YES
29	a	243.30	0.79741	YES	YES
30	a	264.70	1.09374	YES	YES
31	a	280.06	1.21745	YES	YES
32	a	283.52	4.52251	YES	YES
33	a	355.23	1.65612	YES	YES
34	a	368.43	10.41136	YES	YES
35	a	371.16	17.81186	YES	YES
36	a	409.54	9.00014	YES	YES
37	a	420.83	0.00760	YES	YES
38	a	432.92	1.90686	YES	YES
39	a	448.63	5.06107	YES	YES
40	a	458.25	0.05615	YES	YES
41	a	464.84	0.40177	YES	YES
42	a	476.00	5.71754	YES	YES
43	a	482.29	1.90114	YES	YES
44	a	493.30	1.86918	YES	YES
45	a	498.67	1.51402	YES	YES
46	a	505.43	25.56968	YES	YES
47	a	512.67	8.91216	YES	YES
48	a	534.45	2.22502	YES	YES
49	a	538.22	10.33803	YES	YES
50	a	548.54	5.78802	YES	YES

TS_{23be}'

SCF Energy (au) BP86/SV(P) -2391.942812015
SCF Energy (au) PBE0/def2-TZVPP -2391.495806536
SCF Energy (au) PBE0/def2-TZVPP -2391.5041329799 (Toluene Correction)
Zero Point Energy (au) 0.3207053
Chemical Potential (kJ mol^{-1}) 692.34
Dispersion Correction (au) PBE0/def2-TZVPP -0.06659232

xyz coordinates
45

Mn	0.8603316	2.3382340	0.6760216
C	0.9379708	2.8134409	2.4240064
C	2.5972322	1.9219831	0.6837214
C	1.2383753	3.9807492	0.0509475
O	1.4943236	5.0284896	-0.3993022
O	3.7314917	1.6393026	0.6929300
O	0.9821245	3.1300685	3.5447706
C	-2.0001052	1.6116006	1.1448314
C	-1.8528766	3.7743982	0.2505319
C	-3.2426123	3.9286207	0.2380344
C	-4.0396691	2.8590150	0.6846638
C	-3.4130628	1.6950717	1.1349044
C	-1.2323193	0.4638250	1.6312906
C	0.1593725	0.4460522	1.2975217
C	0.9491070	-0.6005383	1.8421360
C	0.3982303	-1.5675800	2.6885341
C	-0.9812609	-1.5513558	2.9909768
C	-1.7903207	-0.5429819	2.4581476
H	-1.1942219	4.5826265	-0.1032778
H	-3.6853800	4.8699977	-0.1221602
H	-5.1394155	2.9332059	0.6768765
H	-4.0114237	0.8367251	1.4749357
H	2.0217462	-0.6538559	1.5932197
H	1.0465926	-2.3497724	3.1180270
H	-1.4162982	-2.3185221	3.6519113
H	-2.8597754	-0.5109985	2.7242278
N	-1.2390138	2.6535486	0.6889858
H	0.4719437	2.2253396	-2.2449167
C	0.4880967	1.7815788	-1.2440234
C	0.4524668	0.6049359	-0.6992029
C	0.6761080	-0.7825776	-1.1266604
C	1.1038637	-3.3947654	-2.1684267
C	2.0076121	-2.3538623	-2.4722466
C	1.7857646	-1.0670649	-1.9553061
C	-0.2132866	-1.8444932	-0.8212391
C	-0.0108466	-3.1234504	-1.3391414
O	1.2167345	-4.6758329	-2.6162467
H	2.8885494	-2.5306660	-3.1066706
H	2.4962790	-0.2586425	-2.1904050
H	-1.0849297	-1.6524542	-0.1762487
H	-0.7078168	-3.9463402	-1.1155303
C	2.3137170	-5.0144689	-3.4480481
H	2.1995729	-6.0916702	-3.6844566
H	3.2895722	-4.8568574	-2.9300167
H	2.3074563	-4.4300586	-4.3986280

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-282.68	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	20.94	0.84604	YES	YES
9	a	29.19	0.79127	YES	YES
10	a	45.47	0.13936	YES	YES
11	a	54.95	0.03365	YES	YES
12	a	65.46	0.30469	YES	YES
13	a	69.54	0.04339	YES	YES
14	a	82.63	0.10799	YES	YES
15	a	89.06	0.48148	YES	YES
16	a	96.18	0.65098	YES	YES
17	a	100.10	0.89539	YES	YES
18	a	104.29	0.41734	YES	YES
19	a	119.76	1.61318	YES	YES
20	a	133.23	0.66472	YES	YES
21	a	151.62	0.52672	YES	YES
22	a	160.18	5.85576	YES	YES
23	a	176.79	0.15200	YES	YES
24	a	190.84	1.83338	YES	YES
25	a	217.29	0.68853	YES	YES
26	a	229.68	2.61832	YES	YES
27	a	245.29	0.45810	YES	YES
28	a	266.00	0.50973	YES	YES
29	a	274.25	4.73900	YES	YES
30	a	282.77	0.36243	YES	YES
31	a	356.37	1.42389	YES	YES
32	a	367.34	4.02929	YES	YES
33	a	410.21	3.71430	YES	YES
34	a	411.57	16.17621	YES	YES
35	a	414.46	0.20458	YES	YES
36	a	433.24	4.05431	YES	YES
37	a	447.79	3.75264	YES	YES
38	a	461.59	0.27501	YES	YES
39	a	476.88	7.40511	YES	YES
40	a	481.37	0.22403	YES	YES
41	a	490.38	1.44038	YES	YES
42	a	496.63	4.12182	YES	YES
43	a	503.13	10.48972	YES	YES
44	a	521.41	27.61373	YES	YES
45	a	533.34	2.49739	YES	YES
46	a	537.21	9.83007	YES	YES
47	a	546.83	10.77086	YES	YES
48	a	552.96	7.48015	YES	YES
49	a	559.28	19.86247	YES	YES
50	a	608.71	41.44731	YES	YES

TS_{23be}

SCF Energy (au) BP86/SV(P) -2391.952065529
SCF Energy (au) PBE0/def2-TZVPP -2391.503796793
SCF Energy (au) PBE0/def2-TZVPP -2391.5119222258 (Toluene Correction)
Zero Point Energy (au) 0.3209337
Chemical Potential (kJ mol^{-1}) 692.54
Dispersion Correction (au) PBE0/def2-TZVPP -0.06432154

xyz coordinates
45

Mn	0.8621936	-1.7437725	0.7912015
C	2.0691026	-2.3221484	2.0057398
C	0.3354707	-3.4232205	0.4714875
C	2.0477510	-1.8564604	-0.5663307
O	2.8360809	-1.9745973	-1.4217577
O	-0.0127487	-4.5200114	0.2724205
O	2.8389768	-2.6915675	2.7970921
C	0.7186338	0.8031975	2.3400358
C	2.1364778	1.0577432	0.4858988
C	2.3787566	2.4023179	0.7796241
C	1.7428917	2.9688187	1.8998988
C	0.9075607	2.1655473	2.6776365
C	-0.1123756	-0.1382387	3.0862403
C	-0.3468487	-1.4032020	2.4575729
C	-1.0799262	-2.3732746	3.1945911
C	-1.5781318	-2.0972743	4.4704671
C	-1.3719378	-0.8308322	5.0635798
C	-0.6428491	0.1382771	4.3711397
H	2.6030517	0.5818446	-0.3898668
H	3.0483642	2.9911698	0.1341671
H	1.8951081	4.0295186	2.1584286
H	0.3867636	2.5872098	3.5498997
H	-1.2721714	-3.3628597	2.7460214
H	-2.1328733	-2.8773296	5.0191101
H	-1.7684895	-0.6134081	6.0684463
H	-0.4549848	1.1142585	4.8487020
N	1.3329404	0.2712019	1.2367404
C	-0.7281873	-0.0773813	-1.6978335
C	0.0682062	-0.3445665	-2.8377042
C	-0.1602890	0.2987836	-4.0637801
C	-1.1912045	1.2563263	-4.1786851
C	-1.9875578	1.5500737	-3.0454890
C	-1.7625880	0.8964494	-1.8360872
H	0.8807869	-1.0823544	-2.7715149
H	0.4793908	0.0469182	-4.9224714
O	-1.4906495	1.9459369	-5.3146853
H	-2.7851059	2.3030503	-3.1476681
H	-2.3898731	1.1356930	-0.9621762
C	-0.5628082	-0.7472342	-0.4310331
C	-1.1738842	-1.1609112	0.6325697
H	-2.1688995	-1.4811356	0.9544857
C	-0.7396093	1.6854028	-6.4882063
H	-1.1636778	2.3394228	-7.2766994
H	-0.8310382	0.6206259	-6.8093990
H	0.3402008	1.9319926	-6.3518091

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-227.33	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	19.41	0.41189	YES	YES
9	a	27.78	0.54285	YES	YES
10	a	40.10	0.12463	YES	YES
11	a	54.50	0.43267	YES	YES
12	a	67.65	0.31805	YES	YES
13	a	70.24	0.07862	YES	YES
14	a	86.69	0.50336	YES	YES
15	a	90.08	0.47264	YES	YES
16	a	91.94	1.11787	YES	YES
17	a	100.97	0.83703	YES	YES
18	a	109.03	0.03787	YES	YES
19	a	113.63	0.02923	YES	YES
20	a	123.87	0.95877	YES	YES
21	a	148.01	0.67670	YES	YES
22	a	176.03	0.53732	YES	YES
23	a	181.06	1.33249	YES	YES
24	a	202.81	0.52002	YES	YES
25	a	232.05	0.65903	YES	YES
26	a	233.23	0.92839	YES	YES
27	a	249.69	3.09180	YES	YES
28	a	259.35	0.42038	YES	YES
29	a	278.91	0.18843	YES	YES
30	a	287.88	3.04993	YES	YES
31	a	357.46	1.85353	YES	YES
32	a	367.87	5.71411	YES	YES
33	a	404.64	1.03540	YES	YES
34	a	413.15	1.34921	YES	YES
35	a	422.17	1.05395	YES	YES
36	a	428.34	9.27362	YES	YES
37	a	438.19	0.18566	YES	YES
38	a	449.62	3.72182	YES	YES
39	a	461.50	0.42404	YES	YES
40	a	472.12	2.83535	YES	YES
41	a	479.94	1.51383	YES	YES
42	a	486.82	0.41372	YES	YES
43	a	498.30	1.84853	YES	YES
44	a	507.44	9.78614	YES	YES
45	a	529.46	6.30823	YES	YES
46	a	544.91	28.96894	YES	YES
47	a	545.21	18.42229	YES	YES
48	a	553.60	0.31762	YES	YES
49	a	568.43	45.03624	YES	YES
50	a	610.58	21.48888	YES	YES

TS_{23bf}

SCF Energy (au) BP86/SV(P) -2376.678364254
SCF Energy (au) PBE0/def2-TZVPP -2376.251797975
SCF Energy (au) PBE0/def2-TZVPP -2376.2588756073 (Toluene Correction)
Zero Point Energy (au) 0.2815138
Chemical Potential (kJ mol^{-1}) 593.78
Dispersion Correction (au) PBE0/def2-TZVPP -0.06085022

xyz coordinates
41

Mn	1.5619780	0.3660655	0.7861690
C	1.9208386	0.6208485	2.5404651
C	3.2541360	-0.1276676	0.4770720
C	1.9785849	2.0697894	0.3569203
O	2.2835054	3.1695638	0.1046869
O	4.3562761	-0.4595864	0.2814469
O	2.1400928	0.7768074	3.6726748
C	-1.2440467	-0.2454675	1.5945022
C	-1.0702898	1.9843787	0.8796638
C	-2.4348486	2.2155314	1.0724391
C	-3.2360103	1.1542217	1.5324193
C	-2.6368801	-0.0802472	1.7882012
C	-0.5011196	-1.4767078	1.8553073
C	0.8563183	-1.5017281	1.4009004
C	1.6332937	-2.6484384	1.7196354
C	1.0885552	-3.7252870	2.4242352
C	-0.2647148	-3.7051008	2.8323911
C	-1.0494699	-2.5854594	2.5475681
H	-0.4127089	2.7847534	0.5080550
H	-2.8564114	3.2094672	0.8580455
H	-4.3190959	1.2907115	1.6852720
H	-3.2426676	-0.9298586	2.1358996
H	2.6853571	-2.6982887	1.3913901
H	1.7225618	-4.5955856	2.6642926
H	-0.6941026	-4.5576641	3.3827492
H	-2.0952652	-2.5585120	2.8949469
N	-0.4812431	0.7936973	1.1302499
C	0.3501391	0.6559185	-2.3668529
C	0.9112785	1.8710060	-2.8413999
C	0.4926697	2.4378441	-4.0527881
C	-0.5125640	1.8032486	-4.7954455
C	-1.1025882	0.6096096	-4.3535508
C	-0.6698862	0.0429080	-3.1497629
H	1.6958594	2.3738398	-2.2581371
H	0.9341938	3.3739313	-4.4286426
F	-0.9275114	2.3519564	-5.9545333
H	-1.8929051	0.1390941	-4.9592008
H	-1.1268168	-0.8930985	-2.7913662
C	0.7735382	0.0070599	-1.1487214
C	0.9568754	-1.1398979	-0.5775206
H	1.1704449	-2.1796208	-0.8418947

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-227.53	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-

8	a	19.21	0.24348	YES	YES
9	a	23.75	0.12982	YES	YES
10	a	42.92	0.09885	YES	YES
11	a	56.70	0.11916	YES	YES
12	a	70.27	0.09686	YES	YES
13	a	76.59	0.08731	YES	YES
14	a	88.98	0.27995	YES	YES
15	a	92.03	0.96432	YES	YES
16	a	97.86	0.53452	YES	YES
17	a	108.76	0.12355	YES	YES
18	a	110.28	0.02049	YES	YES
19	a	116.73	0.06153	YES	YES
20	a	146.46	0.79840	YES	YES
21	a	177.78	0.27680	YES	YES
22	a	182.39	1.18811	YES	YES
23	a	205.49	1.46760	YES	YES
24	a	233.38	0.72356	YES	YES
25	a	258.43	0.38635	YES	YES
26	a	275.64	2.52772	YES	YES
27	a	278.75	0.07715	YES	YES
28	a	355.94	2.58164	YES	YES
29	a	363.22	3.60620	YES	YES
30	a	388.27	5.12682	YES	YES
31	a	406.29	2.57962	YES	YES
32	a	411.37	0.41426	YES	YES
33	a	423.31	3.72845	YES	YES
34	a	428.92	4.46412	YES	YES
35	a	445.07	0.06098	YES	YES
36	a	456.35	2.81889	YES	YES
37	a	466.29	6.63396	YES	YES
38	a	475.36	1.39436	YES	YES
39	a	486.90	0.50086	YES	YES
40	a	497.88	4.81588	YES	YES
41	a	504.43	12.18303	YES	YES
42	a	516.93	6.22702	YES	YES
43	a	540.83	14.84431	YES	YES
44	a	543.79	23.93456	YES	YES
45	a	553.24	0.35600	YES	YES
46	a	561.21	22.34925	YES	YES
47	a	611.02	24.09647	YES	YES
48	a	620.17	2.09154	YES	YES
49	a	623.93	31.33547	YES	YES
50	a	628.11	10.34672	YES	YES

TS_{23bf}'

SCF Energy (au) BP86/SV(P) -2376.669021186
SCF Energy (au) PBE0/def2-TZVPP -2376.243801851
SCF Energy (au) PBE0/def2-TZVPP -2376.2510386261 (Toluene Correction)
Zero Point Energy (au) 0.2813228
Chemical Potential (kJ mol^{-1}) 594.57
Dispersion Correction (au) PBE0/def2-TZVPP -0.06310967

xyz coordinates
41

Mn	1.1679605	1.7937775	0.3566876
C	1.3550067	2.1748786	2.1202758
C	2.8948304	1.3467086	0.2513224
C	1.5482691	3.4604883	-0.2019107
O	1.8028072	4.5246093	-0.6113293
O	4.0222238	1.0452474	0.1892069
O	1.4715723	2.4296359	3.2510797
C	-1.6803990	1.1013854	0.9435919
C	-1.5330810	3.3042479	0.1537376
C	-2.9181923	3.4841053	0.2210215
C	-3.7138197	2.4080422	0.6542685
C	-3.0897143	1.2110733	1.0121351
C	-0.9131107	-0.0848258	1.3288097
C	0.4585613	-0.1118585	0.9211469
C	1.2528511	-1.2010783	1.3662344
C	0.7256611	-2.2017573	2.1886064
C	-0.6352314	-2.1751473	2.5649013
C	-1.4485718	-1.1236896	2.1304586
H	-0.8768868	4.1173775	-0.1931761
H	-3.3590507	4.4503817	-0.0685604
H	-4.8107081	2.5029422	0.7075116
H	-3.6879218	0.3476784	1.3392749
H	2.3096177	-1.2610650	1.0582935
H	1.3785562	-3.0180279	2.5406817
H	-1.0517775	-2.9678258	3.2072608
H	-2.5015099	-1.0854712	2.4550728
N	-0.9214283	2.1511209	0.5024351
H	0.6243956	1.8451641	-2.5424786
C	0.6810058	1.3514882	-1.5667166
C	0.6470050	0.1528502	-1.0719944
C	0.8050998	-1.2154115	-1.5896971
C	1.1005693	-3.7481923	-2.7710760
C	2.0104261	-2.7337013	-3.0964077
C	1.8558790	-1.4713673	-2.5055919
C	-0.0902993	-2.2668373	-1.2791782
C	0.0471259	-3.5285723	-1.8715097
F	1.2421296	-4.9643436	-3.3325375
H	2.8286622	-2.9435393	-3.8026004
H	2.5658972	-0.6638700	-2.7434700
H	-0.9133767	-2.0872068	-0.5704353
H	-0.6510337	-4.3494144	-1.6453449

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-281.12	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-

8	a	23.06	0.43019	YES	YES
9	a	33.28	0.22086	YES	YES
10	a	45.13	0.06902	YES	YES
11	a	57.85	0.03442	YES	YES
12	a	65.73	0.24950	YES	YES
13	a	74.52	0.20522	YES	YES
14	a	85.64	0.15124	YES	YES
15	a	90.27	0.39165	YES	YES
16	a	99.81	0.62535	YES	YES
17	a	104.52	0.34564	YES	YES
18	a	110.26	0.08384	YES	YES
19	a	136.48	0.24950	YES	YES
20	a	154.01	0.08206	YES	YES
21	a	167.10	3.25609	YES	YES
22	a	181.48	0.60014	YES	YES
23	a	205.28	1.40959	YES	YES
24	a	218.29	0.72221	YES	YES
25	a	245.32	1.21865	YES	YES
26	a	258.04	2.84291	YES	YES
27	a	281.62	0.30776	YES	YES
28	a	356.45	1.45448	YES	YES
29	a	359.88	1.62025	YES	YES
30	a	403.54	8.10795	YES	YES
31	a	412.41	1.13305	YES	YES
32	a	413.93	0.24644	YES	YES
33	a	430.46	0.39448	YES	YES
34	a	444.28	12.65374	YES	YES
35	a	449.03	11.34976	YES	YES
36	a	460.93	0.31257	YES	YES
37	a	478.37	8.32081	YES	YES
38	a	486.58	11.15331	YES	YES
39	a	492.15	10.15353	YES	YES
40	a	496.96	1.50645	YES	YES
41	a	507.24	2.14471	YES	YES
42	a	531.58	2.35931	YES	YES
43	a	536.44	13.07556	YES	YES
44	a	545.62	3.08104	YES	YES
45	a	552.27	11.54518	YES	YES
46	a	557.93	12.44836	YES	YES
47	a	607.80	42.28800	YES	YES
48	a	619.49	1.47328	YES	YES
49	a	624.35	37.81025	YES	YES
50	a	629.46	2.75821	YES	YES

TS_{23bg}

SCF Energy (au) BP86/SV(P) -2614.321919435
SCF Energy (au) PBE0/def2-TZVPP -2613.938388064
SCF Energy (au) PBE0/def2-TZVPP -2613.9456534346 (Toluene Correction)
Zero Point Energy (au) 0.2938786
Chemical Potential (kJ mol^{-1}) 609.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.06429204

xyz coordinates
44

Mn	1.6199261	0.1839127	1.2244550
C	1.9703585	0.4585406	2.9778204
C	3.3203503	-0.2897316	0.9266841
C	2.0127327	1.8912149	0.7828043
O	2.2972423	2.9925574	0.5179697
O	4.4275292	-0.6078570	0.7384601
O	2.1853940	0.6268440	4.1086720
C	-1.1792486	-0.4538706	2.0373772
C	-1.0355679	1.7700997	1.2989351
C	-2.4029705	1.9850299	1.4916835
C	-3.1890964	0.9188300	1.9654244
C	-2.5732740	-0.3050667	2.2331667
C	-0.4201235	-1.6737136	2.3090137
C	0.9355425	-1.6886456	1.8509875
C	1.7276002	-2.8220221	2.1778069
C	1.2003632	-3.8950022	2.9016578
C	-0.1504308	-3.8841555	3.3175383
C	-0.9510923	-2.7789871	3.0201217
H	-0.3899306	2.5751603	0.9165658
H	-2.8381934	2.9706082	1.2663466
H	-4.2734418	1.0429133	2.1195822
H	-3.1670728	-1.1587135	2.5914871
H	2.7779030	-2.8640172	1.8430276
H	1.8459733	-4.7541239	3.1503903
H	-0.5662476	-4.7332208	3.8834527
H	-1.9950363	-2.7600360	3.3732780
N	-0.4304319	0.5901520	1.5618163
C	0.4252095	0.4646606	-1.9214119
C	1.0845783	1.6109801	-2.4406344
C	0.6668475	2.1973363	-3.6394776
C	-0.4316259	1.6717741	-4.3481923
C	-1.1054294	0.5431403	-3.8415792
C	-0.6837424	-0.0528002	-2.6485551
H	1.9388036	2.0406499	-1.8981213
H	1.1940743	3.0839041	-4.0254955
C	-0.8489076	2.2954447	-5.6585145
H	-1.9705211	0.1313201	-4.3839526
H	-1.2180867	-0.9313327	-2.2533843
C	0.8396665	-0.1949227	-0.7088548
C	1.0375226	-1.3347500	-0.1287520
H	1.2599484	-2.3733239	-0.3917808
F	-0.7199966	3.6466930	-5.6358574
F	-2.1388102	2.0147342	-5.9680578
F	-0.0882877	1.8497925	-6.6939033

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-221.56	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	7.57	0.08787	YES	YES
9	a	12.70	0.02691	YES	YES
10	a	17.57	0.40150	YES	YES
11	a	39.40	0.11062	YES	YES
12	a	53.16	0.26578	YES	YES
13	a	64.57	0.09205	YES	YES
14	a	68.37	0.13503	YES	YES
15	a	84.86	0.30126	YES	YES
16	a	88.58	0.21602	YES	YES
17	a	90.97	0.86229	YES	YES
18	a	101.75	0.61090	YES	YES
19	a	107.00	0.11636	YES	YES
20	a	111.52	0.04179	YES	YES
21	a	123.67	0.39127	YES	YES
22	a	166.48	2.85398	YES	YES
23	a	169.78	0.80858	YES	YES
24	a	189.44	0.55734	YES	YES
25	a	197.50	1.45027	YES	YES
26	a	205.67	1.38839	YES	YES
27	a	234.18	0.76864	YES	YES
28	a	258.19	0.93481	YES	YES
29	a	278.23	0.21455	YES	YES
30	a	294.42	2.80403	YES	YES
31	a	333.91	12.63884	YES	YES
32	a	358.35	1.03901	YES	YES
33	a	383.65	2.02331	YES	YES
34	a	400.39	5.40651	YES	YES
35	a	402.37	1.56811	YES	YES
36	a	411.18	1.44785	YES	YES
37	a	426.61	12.14994	YES	YES
38	a	435.36	0.54616	YES	YES
39	a	455.25	4.11501	YES	YES
40	a	464.66	8.39488	YES	YES
41	a	466.98	0.81202	YES	YES
42	a	476.39	0.76004	YES	YES
43	a	492.10	1.01598	YES	YES
44	a	497.58	11.50701	YES	YES
45	a	502.37	4.21196	YES	YES
46	a	521.29	1.91749	YES	YES
47	a	542.49	12.24062	YES	YES
48	a	545.04	10.18632	YES	YES
49	a	553.10	1.46029	YES	YES
50	a	564.73	0.25262	YES	YES

TS_{23bg}'

SCF Energy (au) BP86/SV(P) -2614.309477147
SCF Energy (au) PBE0/def2-TZVPP -2613.929233249
SCF Energy (au) PBE0/def2-TZVPP -2613.9365857123 (Toluene Correction)
Zero Point Energy (au) 0.2938482
Chemical Potential (kJ mol^{-1}) 615.77
Dispersion Correction (au) PBE0/def2-TZVPP -0.06657179

xyz coordinates
44

Mn	1.0446202	2.2196695	0.5499048
C	1.1981552	2.6359065	2.3093251
C	2.7832881	1.8101785	0.4800956
C	1.3941553	3.8859223	-0.0312781
O	1.6281967	4.9485527	-0.4553341
O	3.9179773	1.5340174	0.4444023
O	1.2902589	2.9124888	3.4368457
C	-1.7905760	1.4788949	1.1355548
C	-1.6847092	3.6702602	0.3070757
C	-3.0724214	3.8273872	0.3775804
C	-3.8472378	2.7460619	0.8344706
C	-3.2011110	1.5661279	1.2096823
C	-1.0016303	0.3123426	1.5382334
C	0.3728925	0.3073319	1.1399938
C	1.1861554	-0.7613311	1.5995115
C	0.6733319	-1.7655737	2.4267004
C	-0.6892004	-1.7600573	2.7968418
C	-1.5198851	-0.7277174	2.3494605
H	-1.0442952	4.4890153	-0.0557742
H	-3.5311239	4.7808319	0.0735908
H	-4.9451686	2.8235315	0.8929761
H	-3.7832541	0.6993749	1.5562845
H	2.2456846	-0.8032007	1.2981667
H	1.3391203	-2.5672179	2.7878006
H	-1.0941491	-2.5549752	3.4437029
H	-2.5744458	-0.7064679	2.6701195
N	-1.0519180	2.5341520	0.6732917
H	0.5631348	2.2112433	-2.3631115
C	0.6037548	1.7379934	-1.3765606
C	0.5771495	0.5524922	-0.8521550
C	0.7362246	-0.8300358	-1.3363065
C	1.0549481	-3.4210172	-2.4309260
C	1.9940182	-2.4157620	-2.7184140
C	1.8324125	-1.1303839	-2.1795329
C	-0.2001407	-1.8529545	-1.0541714
C	-0.0489507	-3.1298277	-1.6038352
C	1.2296801	-4.8283375	-2.9552798
H	2.8553113	-2.6375007	-3.3665245
H	2.5692766	-0.3425361	-2.4007842
H	-1.0604641	-1.6353141	-0.4029020
H	-0.7948139	-3.9112308	-1.3883314
F	1.5905075	-5.6834771	-1.9621783
F	2.1802621	-4.9093161	-3.9162865
F	0.0749786	-5.3095419	-3.4819251

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-255.12	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	19.38	0.35992	YES	YES
9	a	27.80	0.03761	YES	YES
10	a	36.47	0.52845	YES	YES
11	a	39.58	0.21012	YES	YES
12	a	53.23	0.14211	YES	YES
13	a	64.72	0.08135	YES	YES
14	a	68.31	0.41793	YES	YES
15	a	84.55	0.02591	YES	YES
16	a	89.92	0.66128	YES	YES
17	a	98.38	0.68424	YES	YES
18	a	99.94	0.07422	YES	YES
19	a	106.78	0.31950	YES	YES
20	a	114.25	0.24696	YES	YES
21	a	134.60	0.04530	YES	YES
22	a	147.90	0.70488	YES	YES
23	a	158.95	0.91092	YES	YES
24	a	174.99	0.16022	YES	YES
25	a	205.88	0.13288	YES	YES
26	a	222.42	2.44858	YES	YES
27	a	227.63	0.35744	YES	YES
28	a	249.15	0.21159	YES	YES
29	a	278.70	1.18101	YES	YES
30	a	283.25	0.15136	YES	YES
31	a	349.26	9.91686	YES	YES
32	a	359.42	6.76641	YES	YES
33	a	383.55	2.45183	YES	YES
34	a	395.33	2.70311	YES	YES
35	a	398.54	1.47142	YES	YES
36	a	416.19	6.80839	YES	YES
37	a	430.08	0.93652	YES	YES
38	a	447.93	4.21251	YES	YES
39	a	457.31	0.25923	YES	YES
40	a	464.37	2.95976	YES	YES
41	a	475.72	0.71042	YES	YES
42	a	487.97	2.61682	YES	YES
43	a	494.87	3.04247	YES	YES
44	a	509.69	1.79537	YES	YES
45	a	521.65	1.12330	YES	YES
46	a	523.98	8.59362	YES	YES
47	a	536.63	14.48469	YES	YES
48	a	550.84	2.04644	YES	YES
49	a	557.50	1.58670	YES	YES
50	a	570.14	0.27068	YES	YES

TS_{23bh}

SCF Energy (au) BP86/SV(P) -2505.236367416
SCF Energy (au) PBE0/def2-TZVPP -2504.785704894
SCF Energy (au) PBE0/def2-TZVPP -2504.7950366914 (Toluene Correction)
Zero Point Energy (au) 0.3307489
Chemical Potential (kJ mol^{-1}) 706.50
Dispersion Correction (au) PBE0/def2-TZVPP -0.06699044

xyz coordinates
47

Mn	1.6754286	-0.0989474	1.7320687
C	2.0246866	0.1907221	3.4826619
C	3.3761028	-0.5732624	1.4381564
C	2.0663400	1.6058582	1.2761918
O	2.3505924	2.7059428	1.0062560
O	4.4836663	-0.8920963	1.2525671
O	2.2394096	0.3678434	4.6123541
C	-1.1236676	-0.7355322	2.5456355
C	-0.9827449	1.4824181	1.7886419
C	-2.3512267	1.6956683	1.9750354
C	-3.1364053	0.6318319	2.4555878
C	-2.5185919	-0.5881900	2.7359582
C	-0.3629939	-1.9519531	2.8274500
C	0.9942964	-1.9662292	2.3738530
C	1.7871152	-3.0969841	2.7083437
C	1.2591085	-4.1680168	3.4344833
C	-0.0931520	-4.1578398	3.8456843
C	-0.8945836	-3.0551473	3.5412365
H	-0.3378479	2.2853166	1.4005864
H	-2.7881502	2.6779311	1.7388707
H	-4.2216541	0.7544255	2.6044017
H	-3.1116575	-1.4403217	3.0990710
H	2.8387260	-3.1386268	2.3775361
H	1.9051987	-5.0252121	3.6886868
H	-0.5096903	-5.0056651	4.4129586
H	-1.9400714	-3.0369371	3.8898672
N	-0.3756995	0.3062179	2.0637330
C	0.4636371	0.1596775	-1.4108760
C	1.1217846	1.2999242	-1.9468962
C	0.6946638	1.8756950	-3.1472259
C	-0.4168376	1.3493412	-3.8430565
C	-1.0859068	0.2230198	-3.3128248
C	-0.6556187	-0.3642270	-2.1220225
H	1.9853339	1.7276221	-1.4171679
H	1.2213671	2.7505785	-3.5564537
C	-0.9245870	1.9319464	-5.1192142
H	-1.9516267	-0.1796151	-3.8622928
H	-1.1828555	-1.2410020	-1.7133119
C	0.8882290	-0.4932444	-0.2000688
C	1.0969078	-1.6260932	0.3897569
H	1.3282855	-2.6646696	0.1347985
O	-0.1900944	3.0065661	-5.5221740
O	-1.8845255	1.5108534	-5.7466551
C	-0.6152721	3.6178162	-6.7452257
H	-0.5710537	2.8924294	-7.5861685
H	0.0841179	4.4583675	-6.9218394
H	-1.6584831	3.9917998	-6.6589589

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-220.95	0.00000	YES	YES

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	7.19	0.62059	YES	YES
9	a	17.95	0.53375	YES	YES
10	a	33.13	0.60224	YES	YES
11	a	50.45	0.43904	YES	YES
12	a	62.46	0.22710	YES	YES
13	a	65.98	0.05742	YES	YES
14	a	71.16	0.53438	YES	YES
15	a	81.74	0.48049	YES	YES
16	a	88.35	0.37958	YES	YES
17	a	91.20	0.84586	YES	YES
18	a	100.95	0.52271	YES	YES
19	a	104.34	0.18076	YES	YES
20	a	110.48	0.04179	YES	YES
21	a	114.82	0.38083	YES	YES
22	a	122.64	0.13392	YES	YES
23	a	151.79	1.20487	YES	YES
24	a	162.80	2.63536	YES	YES
25	a	172.13	1.96656	YES	YES
26	a	186.96	2.89815	YES	YES
27	a	196.98	0.65384	YES	YES
28	a	234.08	0.43297	YES	YES
29	a	243.10	2.46732	YES	YES
30	a	258.63	1.81873	YES	YES
31	a	278.49	0.18283	YES	YES
32	a	310.30	17.10652	YES	YES
33	a	330.95	7.58735	YES	YES
34	a	357.39	4.72527	YES	YES
35	a	366.76	16.85249	YES	YES
36	a	406.16	0.17136	YES	YES
37	a	410.28	2.19811	YES	YES
38	a	419.15	3.05301	YES	YES
39	a	432.70	3.35204	YES	YES
40	a	444.49	1.07229	YES	YES
41	a	458.63	2.25641	YES	YES
42	a	463.19	6.28765	YES	YES
43	a	468.90	5.35694	YES	YES
44	a	481.86	0.52039	YES	YES
45	a	494.74	3.15862	YES	YES
46	a	502.91	11.21556	YES	YES
47	a	510.39	13.39519	YES	YES
48	a	531.24	6.55006	YES	YES
49	a	544.18	13.64828	YES	YES
50	a	549.57	6.58159	YES	YES

TS_{23bh}'

SCF Energy (au) BP86/SV(P) -2505.225492213
SCF Energy (au) PBE0/def2-TZVPP -2504.775890270
SCF Energy (au) PBE0/def2-TZVPP -2504.7853054603 (Toluene Correction)
Zero Point Energy (au) 0.3306400
Chemical Potential (kJ mol^{-1}) 709.19
Dispersion Correction (au) PBE0/def2-TZVPP -0.06918112

xyz coordinates
47

Mn	0.9887955	2.7402352	0.7706369
C	1.0993447	3.1983377	2.5227002
C	2.7327679	2.3462166	0.7441052
C	1.3325783	4.3975058	0.1610897
O	1.5635823	5.4539063	-0.2801258
O	3.8701017	2.0799175	0.7359770
O	1.1627870	3.5019474	3.6453639
C	-1.8493390	1.9787834	1.3069888
C	-1.7496036	4.1506747	0.4281616
C	-3.1406970	4.2900659	0.4562208
C	-3.9135692	3.2089836	0.9170475
C	-3.2624680	2.0479015	1.3394548
C	-1.0562409	0.8339295	1.7602694
C	0.3267248	0.8359876	1.3934286
C	1.1423542	-0.2092920	1.8991227
C	0.6232379	-1.1958656	2.7438670
C	-0.7471626	-1.1977348	3.0836444
C	-1.5805428	-0.1897356	2.5881098
H	-1.1101961	4.9691260	0.0627906
H	-3.6031842	5.2293250	0.1159073
H	-5.0136938	3.2720352	0.9419270
H	-3.8421898	1.1812040	1.6903115
H	2.2090619	-0.2462592	1.6234060
H	1.2906992	-1.9780785	3.1427249
H	-1.1566153	-1.9788526	3.7444260
H	-2.6425742	-0.1732216	2.8834889
N	-1.1121824	3.0325985	0.8391478
H	0.5731256	2.6691468	-2.1492393
C	0.5999846	2.2146977	-1.1533827
C	0.5725363	1.0374637	-0.6096531
C	0.7569336	-0.3466514	-1.0761748
C	1.1032229	-2.9331540	-2.1894601
C	1.9936720	-1.8902474	-2.5201913
C	1.8227303	-0.6136950	-1.9733878
C	-0.1261273	-1.4013112	-0.7416334
C	0.0391434	-2.6750319	-1.2969620
C	1.3347123	-4.2748564	-2.8077003
H	2.8222398	-2.1055597	-3.2130084
H	2.5225023	0.1981937	-2.2265386
H	-0.9587920	-1.2106318	-0.0473453
H	-0.6601518	-3.4848910	-1.0415122
O	0.4172089	-5.1943266	-2.4003227
O	2.2358853	-4.5350583	-3.5888433
C	0.5740883	-6.5059498	-2.9548469
H	1.5647993	-6.9322792	-2.6864025
H	0.4918442	-6.4785578	-4.0629580
H	-0.2413344	-7.1169416	-2.5206298

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-279.75	0.00000	YES	YES

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	17.51	0.16059	YES	YES
9	a	24.76	0.87042	YES	YES
10	a	32.68	0.08852	YES	YES
11	a	47.97	0.12715	YES	YES
12	a	64.95	0.28703	YES	YES
13	a	67.25	0.27949	YES	YES
14	a	70.35	0.90578	YES	YES
15	a	82.07	0.00642	YES	YES
16	a	87.39	0.43598	YES	YES
17	a	94.66	0.19779	YES	YES
18	a	100.79	0.72579	YES	YES
19	a	103.57	0.34623	YES	YES
20	a	112.09	1.05407	YES	YES
21	a	118.76	0.83993	YES	YES
22	a	127.62	0.31218	YES	YES
23	a	145.61	0.61791	YES	YES
24	a	153.40	2.18467	YES	YES
25	a	166.37	1.25911	YES	YES
26	a	184.68	2.11024	YES	YES
27	a	213.11	0.34696	YES	YES
28	a	220.16	0.27071	YES	YES
29	a	238.70	4.94535	YES	YES
30	a	250.11	1.12507	YES	YES
31	a	280.11	0.16457	YES	YES
32	a	311.94	19.32206	YES	YES
33	a	342.79	4.65277	YES	YES
34	a	352.63	5.38192	YES	YES
35	a	359.74	5.76677	YES	YES
36	a	406.74	0.90136	YES	YES
37	a	409.68	8.43837	YES	YES
38	a	417.12	3.65096	YES	YES
39	a	439.06	1.80633	YES	YES
40	a	456.81	4.34689	YES	YES
41	a	463.91	1.20800	YES	YES
42	a	472.63	7.62376	YES	YES
43	a	481.41	4.75192	YES	YES
44	a	490.61	0.25573	YES	YES
45	a	496.13	1.41333	YES	YES
46	a	506.21	4.74702	YES	YES
47	a	530.13	5.95655	YES	YES
48	a	533.50	3.73254	YES	YES
49	a	537.58	8.44805	YES	YES
50	a	551.81	5.46093	YES	YES

TS_{23bi}

SCF Energy (au) BP86/SV(P) -2508.400949832
SCF Energy (au) PBE0/def2-TZVPP -2507.915535463
SCF Energy (au) PBE0/def2-TZVPP -2507.9234924354 (Toluene Correction)
Zero Point Energy (au) 0.3685873
Chemical Potential (kJ mol^{-1}) 807.17
Dispersion Correction (au) PBE0/def2-TZVPP -0.08050516

xyz coordinates
51

Mn	1.2284099	1.2096656	1.1382910
C	1.5620366	1.5138190	2.8913023
C	2.9273281	0.7258085	0.8612965
C	1.6434711	2.9064109	0.6896087
O	1.9471210	4.0056210	0.4325857
O	4.0370505	0.4075761	0.6800472
O	1.7693929	1.7061248	4.0206092
C	-1.5930377	0.6161711	1.9181808
C	-1.4230210	2.8073479	1.0951993
C	-2.7945880	3.0321862	1.2429397
C	-3.5965644	1.9873808	1.7374686
C	-2.9914033	0.7740528	2.0703341
C	-0.8419187	-0.5904372	2.2596235
C	0.5137302	-0.6407273	1.7988529
C	1.3020194	-1.7491283	2.2092470
C	0.7803488	-2.7527792	3.0305000
C	-0.5687414	-2.7094054	3.4470207
C	-1.3732091	-1.6351007	3.0566399
H	-0.7646249	3.5942705	0.6972160
H	-3.2206584	4.0087476	0.9665788
H	-4.6845633	2.1190964	1.8557951
H	-3.5965492	-0.0653700	2.4436361
H	2.3484940	-1.8228908	1.8712361
H	1.4288366	-3.5857440	3.3501090
H	-0.9813079	-3.5064344	4.0865512
H	-2.4159104	-1.5845359	3.4112702
N	-0.8284099	1.6382384	1.4219360
C	0.0945543	1.4033769	-2.0120869
C	0.6987102	2.5846759	-2.5170173
C	0.3105255	3.1154749	-3.7557732
C	-0.7014314	2.4984187	-4.5124083
C	-1.3199512	1.3340049	-4.0200295
C	-0.9286343	0.7904781	-2.7899662
H	1.4879791	3.0825054	-1.9351974
H	0.8025534	4.0277355	-4.1325043
H	-1.0100169	2.9242965	-5.4814419
H	-2.1159919	0.8413282	-4.6032712
H	-1.4131168	-0.1221004	-2.4074074
C	0.4849326	0.7919926	-0.7596752
C	0.6176539	-0.3872074	-0.2165945
C	0.9050220	-1.7370470	-0.7305169
C	1.4063271	-4.2630888	-1.9051931
C	2.2618486	-3.1800486	-2.1697585
C	2.0123522	-1.9246944	-1.5928466
C	0.0578509	-2.8380240	-0.4608263
C	0.3020509	-4.0862243	-1.0522565
H	1.6003697	-5.2471813	-2.3632658
H	3.1321351	-3.3104977	-2.8343011
H	2.6808079	-1.0744638	-1.8002598
H	-0.8045580	-2.7030931	0.2113908
H	-0.3757043	-4.9305813	-0.8428687

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-211.54	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	16.37	0.10076	YES	YES
9	a	21.57	0.08172	YES	YES
10	a	34.25	0.18295	YES	YES
11	a	36.01	0.54213	YES	YES
12	a	45.41	0.04774	YES	YES
13	a	59.27	0.17249	YES	YES
14	a	60.78	0.21687	YES	YES
15	a	72.34	0.06198	YES	YES
16	a	82.06	0.05727	YES	YES
17	a	90.47	0.01476	YES	YES
18	a	97.63	0.96153	YES	YES
19	a	100.50	0.54914	YES	YES
20	a	109.58	0.14237	YES	YES
21	a	119.03	0.26936	YES	YES
22	a	134.60	0.28199	YES	YES
23	a	163.90	1.12153	YES	YES
24	a	169.91	0.74455	YES	YES
25	a	182.93	0.83635	YES	YES
26	a	195.42	2.51480	YES	YES
27	a	222.37	2.35535	YES	YES
28	a	228.13	0.18482	YES	YES
29	a	246.98	1.73153	YES	YES
30	a	254.70	0.90979	YES	YES
31	a	282.61	0.22690	YES	YES
32	a	357.35	1.85677	YES	YES
33	a	376.57	1.37678	YES	YES
34	a	386.15	5.82901	YES	YES
35	a	402.20	0.10506	YES	YES
36	a	403.17	0.31570	YES	YES
37	a	416.22	4.47644	YES	YES
38	a	433.54	0.99814	YES	YES
39	a	438.89	1.17057	YES	YES
40	a	458.10	0.65946	YES	YES
41	a	471.77	1.49662	YES	YES
42	a	475.05	1.42520	YES	YES
43	a	491.89	0.85399	YES	YES
44	a	497.24	0.46976	YES	YES
45	a	503.12	0.85840	YES	YES
46	a	522.33	51.85901	YES	YES
47	a	537.37	6.88208	YES	YES
48	a	545.03	6.98089	YES	YES
49	a	552.23	0.60839	YES	YES
50	a	558.89	6.15442	YES	YES

TS_{23bj}

SCF Energy (au) BP86/SV(P) -2360.864038348
SCF Energy (au) PBE0/def2-TZVPP -2360.429227641
SCF Energy (au) PBE0/def2-TZVPP -2360.4352858128 (Toluene Correction)
Zero Point Energy (au) 0.4312018
Chemical Potential (kJ mol^{-1}) 963.71
Dispersion Correction (au) PBE0/def2-TZVPP -0.07320480

xyz coordinates
55

Mn	1.1107140	1.2303049	1.3664159
C	1.4536300	1.4391606	3.1321289
C	2.8216825	0.8326776	1.0473399
C	1.4253820	2.9528506	0.9656235
O	1.6383710	4.0679819	0.6816749
O	3.9410779	0.5625425	0.8435184
O	1.6673532	1.5794104	4.2692846
C	-1.6730865	0.4395534	2.1100267
C	-1.6057870	2.7156785	1.5460238
C	-2.9832332	2.8642757	1.7337919
C	-3.7346329	1.7350554	2.1086907
C	-3.0747851	0.5186962	2.2928447
C	-0.8665972	-0.7623583	2.3160031
C	0.4756185	-0.7158966	1.8125509
C	1.3177891	-1.8216256	2.1160740
C	0.8546450	-2.9182694	2.8506572
C	-0.4826357	-2.9653252	3.3041323
C	-1.3333770	-1.8882625	3.0373132
H	-0.9843578	3.5731816	1.2442892
H	-3.4533714	3.8483478	1.5829998
H	-4.8252653	1.8056594	2.2523417
H	-3.6384380	-0.3837800	2.5721509
H	2.3676456	-1.8105518	1.7788899
H	1.5448939	-3.7457250	3.0870740
H	-0.8465513	-3.8300140	3.8820871
H	-2.3633460	-1.9043005	3.4300284
N	-0.9591051	1.5423094	1.7231250
C	0.1966399	1.7365319	-1.7972506
C	0.3998843	0.9469695	-0.5521279
C	0.4971635	-0.2772839	-0.1349112
C	0.6203960	-1.6273671	-0.7939240
H	0.8380856	-1.4284989	-1.8701320
C	-0.6203238	-2.5383279	-0.6982553
H	1.5056578	-2.1689530	-0.3929317
H	-0.8285708	-2.7767922	0.3683386
C	-0.4533369	-3.8450511	-1.4918898
H	-1.5094005	-1.9814157	-1.0763700
C	-1.6815875	-4.7616080	-1.4184072
H	0.4416387	-4.3915483	-1.1109637
H	-0.2312817	-3.6059767	-2.5592191
H	-1.9058287	-5.0516221	-0.3672155
H	-1.5273465	-5.6969813	-2.0005963
H	-2.5876713	-4.2585816	-1.8259528
C	1.5184950	2.1420550	-2.4916082
H	-0.4194166	1.1371300	-2.5106304
H	-0.3910740	2.6606134	-1.5826174
H	2.1366295	2.7389659	-1.7842564
C	1.2940266	2.9459554	-3.7821047
H	2.1069365	1.2223677	-2.7176136
C	2.6003986	3.3476417	-4.4796392
H	0.7021094	3.8614864	-3.5442694
H	0.6646045	2.3496998	-4.4845199

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H     3.2350785    3.9776542   -3.8167756
H     2.4033074    3.9279319   -5.4080876
H     3.2005533    2.4534281   -4.7631495

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)       km/mol         IR     RAMAN
     1        a            -219.60        0.00000       YES     YES
     2                        0.00        0.00000        -       -
     3                        0.00        0.00000        -       -
     4                        0.00        0.00000        -       -
     5                        0.00        0.00000        -       -
     6                        0.00        0.00000        -       -
     7                        0.00        0.00000        -       -
     8        a               6.59        0.16626       YES     YES
     9        a              21.63        0.11480       YES     YES
    10        a              27.79        0.04135       YES     YES
    11        a              45.37        0.12128       YES     YES
    12        a              53.12        0.02177       YES     YES
    13        a              55.97        0.43534       YES     YES
    14        a              70.10        0.04223       YES     YES
    15        a              72.42        0.08127       YES     YES
    16        a              75.44        0.02293       YES     YES
    17        a              87.47        0.13587       YES     YES
    18        a              96.79        0.38697       YES     YES
    19        a              98.81        0.56577       YES     YES
    20        a             104.77        0.10079       YES     YES
    21        a             106.36        0.13085       YES     YES
    22        a             109.55        0.09909       YES     YES
    23        a             114.55        0.02645       YES     YES
    24        a             127.64        0.56038       YES     YES
    25        a             135.37        0.27014       YES     YES
    26        a             162.64        0.01310       YES     YES
    27        a             175.25        0.25308       YES     YES
    28        a             194.71        1.23061       YES     YES
    29        a             212.94        1.39155       YES     YES
    30        a             228.42        0.21344       YES     YES
    31        a             232.84        0.76318       YES     YES
    32        a             244.25        0.06565       YES     YES
    33        a             248.97        0.13199       YES     YES
    34        a             266.74        0.19040       YES     YES
    35        a             288.27        0.59620       YES     YES
    36        a             295.77        0.89610       YES     YES
    37        a             340.12        0.37202       YES     YES
    38        a             357.71        1.07517       YES     YES
    39        a             374.57        0.06299       YES     YES
    40        a             407.13        1.47999       YES     YES
    41        a             421.35        4.57145       YES     YES
    42        a             432.67        2.39157       YES     YES
    43        a             445.43        1.55153       YES     YES
    44        a             454.74        4.98736       YES     YES
    45        a             466.89        5.00115       YES     YES
    46        a             476.97        1.20250       YES     YES
    47        a             494.06        1.72617       YES     YES
    48        a             501.73        6.91228       YES     YES
    49        a             506.03        1.37450       YES     YES
    50        a             539.27        6.90485       YES     YES
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TS_{23ca}

SCF Energy (au) BP86/SV(P) -2678.188164496
SCF Energy (au) PBE0/def2-TZVPP -2677.701903263
SCF Energy (au) PBE0/def2-TZVPP -2677.7129455643 (Toluene Correction)
Zero Point Energy (au) 0.4155167
Chemical Potential (kJ mol^{-1}) 916.38
Dispersion Correction (au) PBE0/def2-TZVPP -0.08439631

xyz coordinates
57

Mn	0.9098750	1.8356666	-0.2916640
C	1.2396347	1.7871900	1.4765609
C	2.6475571	1.4826921	-0.6359753
C	1.2684348	3.6041827	-0.4316902
O	1.5234693	4.7442112	-0.4771170
O	3.7804513	1.3542633	-0.8649219
O	1.4479138	1.7134857	2.6212918
C	-1.8802210	1.0356747	0.3493143
C	-1.7800896	3.3400611	-0.0736442
C	-3.1543107	3.4950630	0.1368629
C	-3.9182654	2.3601831	0.4620128
C	-3.2752138	1.1242711	0.5635844
C	-1.0968017	-0.1954282	0.4200711
C	0.2443544	-0.0788298	0.0221512
C	1.1020101	-1.2669893	0.0707704
N	0.5215603	-2.4547193	0.6223414
C	-0.8134899	-2.5505430	0.9935413
C	-1.6291399	-1.4425809	0.8747245
O	2.2686222	-1.2951855	-0.3465440
C	-1.3307536	-3.8699686	1.5038338
N	-1.1477021	2.1506025	0.0307723
C	-0.2902579	2.7328610	-3.3445501
C	0.3587554	3.9618873	-3.6353746
C	-0.1252227	4.8024539	-4.6468580
C	-1.2719680	4.4519655	-5.3818446
C	-1.9313876	3.2424671	-5.0980075
C	-1.4509279	2.3912803	-4.0941614
C	0.1940592	1.8083271	-2.3515034
C	0.4807960	0.6193957	-1.9634753
H	-1.1527441	4.2049584	-0.3367287
H	-3.6108193	4.4924433	0.0431678
H	-5.0045652	2.4403470	0.6306485
H	-3.8477972	0.2165580	0.8036044
H	-2.6803769	-1.5363013	1.1820166
H	1.2573669	4.2480346	-3.0692580
H	0.4019777	5.7466836	-4.8629965
H	-1.6512502	5.1200554	-6.1726422
H	-2.8320578	2.9567922	-5.6672691
H	-1.9685037	1.4439589	-3.8730518
H	0.8582417	-0.3508818	-2.3010040
H	-2.3920439	-3.7659231	1.8075188
H	-0.7512141	-4.2328524	2.3812089
H	-1.2788372	-4.6654035	0.7251127
C	1.4364970	-3.5980294	0.7741268
C	1.8947015	-3.8576669	2.2018580
H	2.3122862	-3.3335121	0.1421400
H	0.9677445	-4.5078727	0.3462925
C	2.8641164	-4.3778490	4.8109069
C	2.6104896	-5.4404944	3.9273811
C	2.1261966	-5.1802333	2.6345091
C	2.1530863	-2.7975710	3.0957061
C	2.6320497	-3.0567575	4.3904190

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H     3.2410988   -4.5788708    5.8274084
H     2.7857707   -6.4813136    4.2470369
H     1.9267051   -6.0209632    1.9470027
H     1.9802871   -1.7558425    2.7791501
H     2.8298523   -2.2154333    5.0752334

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol          IR     RAMAN
     1        a            -158.39         0.00000       YES     YES
     2                        0.00         0.00000        -       -
     3                        0.00         0.00000        -       -
     4                        0.00         0.00000        -       -
     5                        0.00         0.00000        -       -
     6                        0.00         0.00000        -       -
     7                        0.00         0.00000        -       -
     8        a              16.31         0.16610       YES     YES
     9        a              19.21         0.14140       YES     YES
    10        a              20.70         0.05217       YES     YES
    11        a              24.15         0.13533       YES     YES
    12        a              28.69         0.60836       YES     YES
    13        a              43.50         0.11576       YES     YES
    14        a              55.93         2.17310       YES     YES
    15        a              70.63         0.18942       YES     YES
    16        a              75.08         0.18011       YES     YES
    17        a              83.27         0.01423       YES     YES
    18        a              85.27         0.56858       YES     YES
    19        a              97.48         0.55006       YES     YES
    20        a             103.95         0.30751       YES     YES
    21        a             111.46         0.39234       YES     YES
    22        a             115.39         0.63150       YES     YES
    23        a             126.26         0.45633       YES     YES
    24        a             145.84         0.24780       YES     YES
    25        a             153.38         0.50353       YES     YES
    26        a             162.83         0.10641       YES     YES
    27        a             192.28         0.83006       YES     YES
    28        a             192.55         0.52243       YES     YES
    29        a             204.96         1.16647       YES     YES
    30        a             213.33         0.26692       YES     YES
    31        a             245.14         0.49944       YES     YES
    32        a             252.28         0.39293       YES     YES
    33        a             255.49         0.28550       YES     YES
    34        a             260.15         1.10096       YES     YES
    35        a             305.23         0.85843       YES     YES
    36        a             326.12         2.04965       YES     YES
    37        a             350.42         7.12781       YES     YES
    38        a             368.62         4.52977       YES     YES
    39        a             383.52         3.78026       YES     YES
    40        a             400.95         0.02287       YES     YES
    41        a             401.52         0.22387       YES     YES
    42        a             411.81        10.99243       YES     YES
    43        a             430.02         7.43046       YES     YES
    44        a             440.22        13.87203       YES     YES
    45        a             450.45        13.59888       YES     YES
    46        a             460.14         1.30985       YES     YES
    47        a             464.12         4.29608       YES     YES
    48        a             468.65         9.67586       YES     YES
    49        a             478.93         0.85227       YES     YES
    50        a             492.04         2.00409       YES     YES
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TS_{23ca}'

SCF Energy (au) BP86/SV(P) -2678.177478525
SCF Energy (au) PBE0/def2-TZVPP -2677.690686045
SCF Energy (au) PBE0/def2-TZVPP -2677.7015428126 (Toluene Correction)
Zero Point Energy (au) 0.4152541
Chemical Potential (kJ mol^{-1}) 916.57
Dispersion Correction (au) PBE0/def2-TZVPP -0.08703529

xyz coordinates
57

Mn	0.7138071	2.8980516	-0.5336869
C	1.1068390	2.9124074	1.2304921
C	2.4330774	2.5191573	-0.9176994
C	1.0673393	4.6427539	-0.8047677
O	1.2919132	5.7699489	-1.0160662
O	3.5587450	2.3776686	-1.1815661
O	1.3553517	2.9018747	2.3702301
C	-2.1057198	2.1386502	0.1223057
C	-1.9501941	4.4577347	-0.1693790
C	-3.3216873	4.6340174	0.0451723
C	-4.1161799	3.4991076	0.2881568
C	-3.5023884	2.2449093	0.3223966
C	-1.3448304	0.8924277	0.1766645
C	-0.0125015	0.9761958	-0.2680189
C	0.8685198	-0.1849968	-0.0775572
N	0.2665812	-1.3659019	0.4587460
C	-1.0716427	-1.4466455	0.8181379
C	-1.8769306	-0.3308541	0.6869901
O	2.0773055	-0.1866064	-0.3435158
C	-1.6044607	-2.7531520	1.3442330
N	-1.3467834	3.2502233	-0.1343219
H	-0.1032397	3.4828033	-3.3241380
C	0.0146097	2.8232305	-2.4592061
C	0.0568635	1.5599712	-2.1817017
H	-1.2997601	5.3214130	-0.3769251
H	-3.7533767	5.6464581	0.0168647
H	-5.2027305	3.5943436	0.4475574
H	-4.0977751	1.3370573	0.4986173
H	-2.9203268	-0.4004872	1.0261529
C	0.1335619	0.2634315	-2.8797375
H	-2.6641268	-2.6326257	1.6477354
H	-1.0283502	-3.1150192	2.2242253
H	-1.5641031	-3.5554622	0.5720072
C	1.1742491	-2.5126875	0.6429649
C	1.6278683	-2.7425968	2.0771552
H	2.0556937	-2.2718138	0.0110307
H	0.6944240	-3.4261753	0.2371900
C	2.5715018	-3.2122539	4.7051519
C	2.2125776	-4.2920695	3.8813847
C	1.7410718	-4.0560628	2.5787635
C	1.9956023	-1.6648834	2.9105629
C	2.4601761	-1.8991837	4.2149380
H	2.9379800	-3.3932633	5.7292854
H	2.2948495	-5.3264140	4.2551135
H	1.4581802	-4.9098036	1.9380594
H	1.9264470	-0.6309753	2.5351710
H	2.7442427	-1.0452621	4.8521320
C	0.2436835	-2.1439634	-4.3543183
C	1.4121581	-1.3909553	-4.1411569
C	1.3624037	-0.1939805	-3.4101481
C	-1.0348033	-0.5068422	-3.0829668
C	-0.9801775	-1.6970952	-3.8257625

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H     0.2866425   -3.0809266   -4.9343947
H     2.3755773   -1.7373742   -4.5504159
H     2.2753711    0.3951156   -3.2379028
H    -1.9912614   -0.1537877   -2.6662400
H    -1.9018648   -2.2788318   -3.9939954

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)      km/mol          IR     RAMAN
     1        a            -281.77       0.00000       YES     YES
     2                        0.00       0.00000        -       -
     3                        0.00       0.00000        -       -
     4                        0.00       0.00000        -       -
     5                        0.00       0.00000        -       -
     6                        0.00       0.00000        -       -
     7                        0.00       0.00000        -       -
     8        a              16.92       0.11677       YES     YES
     9        a              22.81       0.48793       YES     YES
    10        a              23.35       0.50714       YES     YES
    11        a              27.88       0.38305       YES     YES
    12        a              35.47       0.34503       YES     YES
    13        a              41.64       0.12674       YES     YES
    14        a              45.75       0.06490       YES     YES
    15        a              64.64       1.23398       YES     YES
    16        a              79.99       0.08681       YES     YES
    17        a              81.42       0.30846       YES     YES
    18        a              86.23       0.18885       YES     YES
    19        a              86.86       2.02877       YES     YES
    20        a             100.20       0.10912       YES     YES
    21        a             112.65       1.15652       YES     YES
    22        a             117.48       0.75015       YES     YES
    23        a             127.85       0.27572       YES     YES
    24        a             145.38       0.60008       YES     YES
    25        a             159.80       0.21392       YES     YES
    26        a             176.84       5.07115       YES     YES
    27        a             185.84       0.24957       YES     YES
    28        a             191.89       0.82374       YES     YES
    29        a             198.90       2.00031       YES     YES
    30        a             206.45       2.92257       YES     YES
    31        a             229.40       0.29347       YES     YES
    32        a             239.23       0.17811       YES     YES
    33        a             250.82       0.28528       YES     YES
    34        a             260.98       0.06373       YES     YES
    35        a             293.01       0.12201       YES     YES
    36        a             319.69       4.39261       YES     YES
    37        a             337.75       4.13786       YES     YES
    38        a             364.47       3.52406       YES     YES
    39        a             387.66       2.19276       YES     YES
    40        a             400.14       0.42898       YES     YES
    41        a             401.41       0.15064       YES     YES
    42        a             426.70       1.66304       YES     YES
    43        a             441.21      13.80089       YES     YES
    44        a             447.88       0.16682       YES     YES
    45        a             456.14       2.72252       YES     YES
    46        a             463.93       2.63819       YES     YES
    47        a             466.75       2.08337       YES     YES
    48        a             478.66       1.74876       YES     YES
    49        a             489.42       2.32141       YES     YES
    50        a             498.68       7.04635       YES     YES
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TS_{23da}

SCF Energy (au) BP86/SV(P) -2408.995112972
SCF Energy (au) PBE0/def2-TZVPP -2408.528811114
SCF Energy (au) PBE0/def2-TZVPP -2408.5368518917 (Toluene Correction)
Zero Point Energy (au) 0.3176652
Chemical Potential (kJ mol^{-1}) 684.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.06668154

xyz coordinates
45

Mn	1.7275223	0.7999167	0.3898309
C	2.0895483	1.0816028	2.1407390
C	3.4216148	0.2952688	0.0980376
C	2.1216996	2.5065434	-0.0548414
O	2.3942681	3.6123101	-0.3122392
O	4.5224521	-0.0452347	-0.0826326
O	2.3138259	1.2506852	3.2695325
C	-1.0696555	0.1494737	1.1735573
C	-0.9452402	2.3772016	0.4726763
C	-2.3206936	2.5655412	0.6310084
C	-3.0971991	1.4675657	1.0421106
C	-2.4752166	0.2452548	1.3058193
N	-0.3278659	-0.9901403	1.4304791
C	1.0302861	-1.0331570	0.9837798
C	1.5669268	-2.2391538	1.4195374
C	0.5609475	-2.9614117	2.1463357
C	-0.6310173	-2.1594269	2.1567726
H	-0.3007874	3.1946902	0.1159326
H	-2.7694426	3.5462976	0.4137220
H	-4.1910040	1.5577266	1.1436460
H	-3.0675080	-0.6361346	1.5774146
H	2.5910470	-2.5809008	1.2200111
C	-1.7803764	-2.5716864	2.8541962
N	-0.3242258	1.2063843	0.7356993
C	0.6087933	1.1297135	-2.7764697
C	1.3596298	2.2162507	-3.2967806
C	0.9857201	2.8322139	-4.4990762
C	-0.1538459	2.4000883	-5.2007365
C	-0.9146119	1.3319305	-4.6916026
C	-0.5397590	0.7000288	-3.4987574
H	2.2522018	2.5678695	-2.7584966
H	1.5912388	3.6665749	-4.8906988
H	-0.4499531	2.8952950	-6.1401784
H	-1.8107552	0.9834489	-5.2321667
H	-1.1366376	-0.1372632	-3.1019966
C	0.9754901	0.4321249	-1.5662732
C	1.1101977	-0.7218231	-1.0021441
H	1.2974738	-1.7667095	-1.2600597
C	-1.7454693	-3.8123328	3.5148773
H	-2.6863943	-1.9549698	2.9228964
H	-2.6384791	-4.1486237	4.0663696
C	-0.5891616	-4.6246356	3.4900499
H	-0.5951833	-5.5931240	4.0167712
C	0.5654396	-4.2057824	2.8175284
H	1.4741595	-4.8294912	2.8158191

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-237.37	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	16.90	0.00794	YES	YES
9	a	27.26	0.08611	YES	YES
10	a	33.16	0.11095	YES	YES
11	a	54.27	0.16625	YES	YES
12	a	68.89	0.30671	YES	YES
13	a	73.22	0.49740	YES	YES
14	a	76.42	0.13529	YES	YES
15	a	84.67	0.22794	YES	YES
16	a	93.42	0.06507	YES	YES
17	a	100.15	0.60557	YES	YES
18	a	107.55	0.04497	YES	YES
19	a	128.61	0.17288	YES	YES
20	a	137.13	0.25235	YES	YES
21	a	158.03	4.13126	YES	YES
22	a	169.02	0.72987	YES	YES
23	a	200.40	1.72411	YES	YES
24	a	211.16	2.18243	YES	YES
25	a	236.27	3.70321	YES	YES
26	a	239.25	2.39867	YES	YES
27	a	250.95	1.06395	YES	YES
28	a	300.23	1.10439	YES	YES
29	a	336.42	8.93386	YES	YES
30	a	362.82	4.04049	YES	YES
31	a	364.60	3.32119	YES	YES
32	a	400.79	6.52216	YES	YES
33	a	402.21	0.08097	YES	YES
34	a	425.77	8.35193	YES	YES
35	a	433.33	1.36559	YES	YES
36	a	451.84	7.72534	YES	YES
37	a	467.18	1.43404	YES	YES
38	a	482.53	1.07415	YES	YES
39	a	489.01	7.91623	YES	YES
40	a	497.36	1.87821	YES	YES
41	a	502.11	2.52264	YES	YES
42	a	513.86	2.19350	YES	YES
43	a	528.63	4.72170	YES	YES
44	a	536.72	19.06779	YES	YES
45	a	546.95	16.32610	YES	YES
46	a	566.74	0.55150	YES	YES
47	a	573.19	9.51230	YES	YES
48	a	590.52	8.76627	YES	YES
49	a	605.37	8.55967	YES	YES
50	a	611.88	3.41869	YES	YES

TS_{23da}'

SCF Energy (au) BP86/SV(P) -2408.986641492
SCF Energy (au) PBE0/def2-TZVPP -2408.520986012
SCF Energy (au) PBE0/def2-TZVPP -2408.5290620226 (Toluene Correction)
Zero Point Energy (au) 0.3174132
Chemical Potential (kJ mol^{-1}) 684.77
Dispersion Correction (au) PBE0/def2-TZVPP -0.06880878

xyz coordinates
45

Mn	1.3929405	2.1179321	0.0346053
C	1.5920354	2.4758324	1.8024534
C	3.1193805	1.6611721	-0.0761235
C	1.7583553	3.8001150	-0.4949705
O	1.9946440	4.8771940	-0.8799786
O	4.2431992	1.3514463	-0.1390355
O	1.7222591	2.7126864	2.9351880
C	-1.4348519	1.3721376	0.6037112
C	-1.3380177	3.5979133	-0.0999468
C	-2.7269111	3.7407853	-0.0340012
C	-3.4928823	2.6191133	0.3312722
C	-2.8484693	1.4195798	0.6425246
N	-0.6766299	0.2559087	0.9168210
C	0.7030024	0.2367931	0.5363423
C	1.2498842	-0.9340909	1.0457297
C	0.2394481	-1.6424615	1.7795163
C	-0.9732203	-0.8764538	1.7014801
H	-0.6975913	4.4361886	-0.4145309
H	-3.1929470	4.7058657	-0.2834772
H	-4.5933515	2.6730763	0.3596596
H	-3.4263285	0.5176568	0.8777316
H	2.2870153	-1.2597861	0.8958340
C	-2.1347038	-1.2771142	2.3859537
N	-0.6966783	2.4499950	0.2097932
H	0.8708690	2.2675579	-2.8666379
C	0.9239950	1.7187705	-1.9211631
C	0.8921691	0.5014069	-1.4887468
C	1.0615201	-0.8629432	-2.0061543
C	-2.0883262	-2.4734346	3.1229722
H	-3.0576234	-0.6815185	2.3865140
H	-2.9892199	-2.8001588	3.6674636
C	-0.9111694	-3.2539717	3.1835882
H	-0.9094097	-4.1884285	3.7685879
C	0.2537007	-2.8445431	2.5232639
H	1.1781725	-3.4410599	2.5878421
C	1.3873297	-3.4133154	-3.1850301
C	2.3456125	-2.4095796	-3.4036839
C	2.1833224	-1.1409638	-2.8239487
C	0.1079126	-1.8843728	-1.7845339
C	0.2664994	-3.1444326	-2.3776991
H	1.5134272	-4.4086686	-3.6423504
H	3.2295294	-2.6135106	-4.0305493
H	2.9334823	-0.3513558	-2.9890131
H	-0.7698230	-1.6806500	-1.1517711
H	-0.4915512	-3.9263131	-2.2055020

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-287.82	0.00000	YES	YES
2		0.00	0.00000	-	-

3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	20.67	0.60655	YES	YES
9	a	28.74	0.41890	YES	YES
10	a	42.36	0.06185	YES	YES
11	a	48.42	0.04076	YES	YES
12	a	62.97	0.44129	YES	YES
13	a	71.63	0.08685	YES	YES
14	a	77.65	0.26895	YES	YES
15	a	86.77	0.22815	YES	YES
16	a	89.66	0.18222	YES	YES
17	a	96.58	0.02826	YES	YES
18	a	102.25	0.40104	YES	YES
19	a	131.02	0.25623	YES	YES
20	a	132.36	0.74006	YES	YES
21	a	161.35	2.79207	YES	YES
22	a	176.38	7.58770	YES	YES
23	a	197.25	1.11695	YES	YES
24	a	205.64	1.84132	YES	YES
25	a	228.37	3.45227	YES	YES
26	a	233.19	0.79052	YES	YES
27	a	255.52	1.79123	YES	YES
28	a	300.11	0.94208	YES	YES
29	a	326.31	4.03321	YES	YES
30	a	363.15	4.81019	YES	YES
31	a	367.03	1.79414	YES	YES
32	a	402.97	0.07985	YES	YES
33	a	416.28	5.42703	YES	YES
34	a	433.86	0.86468	YES	YES
35	a	456.32	1.84925	YES	YES
36	a	458.93	1.96833	YES	YES
37	a	474.37	5.79367	YES	YES
38	a	484.31	0.73568	YES	YES
39	a	493.32	9.72999	YES	YES
40	a	497.86	19.72214	YES	YES
41	a	504.56	1.35928	YES	YES
42	a	516.71	2.70257	YES	YES
43	a	530.08	20.04411	YES	YES
44	a	538.14	5.12531	YES	YES
45	a	554.22	11.05044	YES	YES
46	a	555.69	18.32082	YES	YES
47	a	567.67	1.46299	YES	YES
48	a	591.43	10.61040	YES	YES
49	a	611.96	3.40366	YES	YES
50	a	613.21	0.62181	YES	YES

TS_{23ea}

SCF Energy (au) BP86/SV(P) -2583.753044495
SCF Energy (au) PBE0/def2-TZVPP -2583.299586047
SCF Energy (au) PBE0/def2-TZVPP -2583.3092723309 (Toluene Correction)
Zero Point Energy (au) 0.3857030
Chemical Potential (kJ mol^{-1}) 843.61
Dispersion Correction (au) PBE0/def2-TZVPP -0.07220089

xyz coordinates
53

Mn	2.3833058	0.8483205	0.3108484
C	2.6727450	1.1691657	2.0615271
C	4.1166155	0.4487440	0.0725329
C	2.6466621	2.5783517	-0.1538424
O	2.8190904	3.7029692	-0.4141811
O	5.2432486	0.1718222	-0.0696683
O	2.8494658	1.3606284	3.1967976
C	-0.4004547	0.1554101	0.9220468
C	-1.8785234	0.2888813	0.9662264
C	0.3311949	-1.0383896	1.3080514
C	1.7274833	-1.0184595	0.9764134
C	2.5353600	-2.1001426	1.4115396
C	1.9793464	-3.1718278	2.1320991
C	0.5878700	-3.1897654	2.4353188
C	-0.2173080	-2.1328742	2.0301947
H	3.6098354	-2.0926353	1.1731258
O	2.6855051	-4.2349131	2.6000951
H	0.1863604	-4.0397473	3.0079205
H	-1.2853858	-2.1288864	2.3014784
N	0.3690596	1.1381350	0.5004391
C	1.2656167	0.9684925	-2.9026942
C	1.7993636	2.1870718	-3.3979245
C	1.3830038	2.7006197	-4.6345102
C	0.4137082	2.0276644	-5.3995675
C	-0.1341568	0.8245695	-4.9168780
C	0.2844428	0.2986441	-3.6880383
H	2.5531545	2.7282996	-2.8080934
H	1.8191197	3.6441258	-5.0027592
H	0.0829049	2.4402888	-6.3669099
H	-0.8972491	0.2883857	-5.5058238
H	-0.1471660	-0.6420084	-3.3100178
C	1.6874677	0.3688457	-1.6591208
C	1.9467988	-0.7307784	-1.0314793
H	2.2581332	-1.7603291	-1.2274445
C	-4.7037107	0.6189425	0.9711380
C	-4.1194987	-0.5712115	0.4755624
C	-2.7333012	-0.7332381	0.4793554
C	-2.4747491	1.4726042	1.4537188
C	-3.8675218	1.6450218	1.4648803
O	-6.0608174	0.6777296	0.9309396
H	-4.7856424	-1.3557750	0.0837907
H	-2.2967469	-1.6576109	0.0685523
H	-1.8356938	2.2731621	1.8627868
H	-4.2889202	2.5770713	1.8687505
H	-0.1328790	1.9651192	0.1475545
C	4.0842964	-4.2897159	2.3632922
C	-6.7122521	1.8464633	1.4041348
H	4.6123053	-3.4217927	2.8227643
H	4.3166356	-4.3214205	1.2730434
H	4.4385375	-5.2266522	2.8382625
H	-6.5048590	2.0246182	2.4856943
H	-7.7977912	1.6687913	1.2676145

H -6.4140099 2.7492149 0.8204629

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-208.55	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	15.47	0.07161	YES	YES
9	a	16.51	0.10232	YES	YES
10	a	33.01	0.47225	YES	YES
11	a	38.56	0.38207	YES	YES
12	a	43.92	0.70894	YES	YES
13	a	46.39	0.32732	YES	YES
14	a	61.18	0.20756	YES	YES
15	a	73.20	0.46680	YES	YES
16	a	75.48	0.18658	YES	YES
17	a	86.94	0.06247	YES	YES
18	a	89.04	0.29431	YES	YES
19	a	97.18	0.31965	YES	YES
20	a	105.22	2.00191	YES	YES
21	a	113.00	0.98813	YES	YES
22	a	125.65	0.79241	YES	YES
23	a	134.73	1.05068	YES	YES
24	a	151.30	1.78706	YES	YES
25	a	160.31	1.44935	YES	YES
26	a	179.53	0.32215	YES	YES
27	a	188.52	0.23415	YES	YES
28	a	197.77	0.33095	YES	YES
29	a	213.48	0.36455	YES	YES
30	a	233.72	0.26149	YES	YES
31	a	241.14	0.49848	YES	YES
32	a	260.07	0.76530	YES	YES
33	a	265.83	2.10419	YES	YES
34	a	297.40	3.78161	YES	YES
35	a	321.18	0.63206	YES	YES
36	a	338.79	4.50691	YES	YES
37	a	342.71	7.05066	YES	YES
38	a	367.37	3.38791	YES	YES
39	a	401.37	1.93286	YES	YES
40	a	402.87	0.12617	YES	YES
41	a	416.51	0.58616	YES	YES
42	a	418.70	2.95551	YES	YES
43	a	435.27	1.24917	YES	YES
44	a	449.98	3.46461	YES	YES
45	a	454.81	2.85799	YES	YES
46	a	468.62	10.92685	YES	YES
47	a	482.98	0.52244	YES	YES
48	a	493.07	3.92736	YES	YES
49	a	499.16	7.85117	YES	YES
50	a	501.98	5.34270	YES	YES

TS_{23ea}'

SCF Energy (au) BP86/SV(P) -2583.738258985
SCF Energy (au) PBE0/def2-TZVPP -2583.285628368
SCF Energy (au) PBE0/def2-TZVPP -2583.2957410864 (Toluene Correction)
Zero Point Energy (au) 0.3849902
Chemical Potential (kJ mol^{-1}) 841.35
Dispersion Correction (au) PBE0/def2-TZVPP -0.07451576

xyz coordinates
53

Mn	2.1746510	1.9645105	-0.4690860
C	2.6450634	2.4259098	1.2145880
C	3.8781896	1.5626495	-0.8563270
C	2.3534054	3.6185339	-1.1566146
O	2.4489731	4.6785438	-1.6355252
O	4.9897225	1.2963138	-1.1038729
O	2.9325961	2.7213873	2.3051651
C	-0.5284013	1.3313376	0.5157799
C	0.2253290	0.1323297	0.8434505
C	1.5604853	0.0882302	0.2933244
C	2.4022337	-0.9653433	0.7115988
C	1.9613766	-1.9532893	1.6126250
C	0.6165517	-1.9494312	2.0721544
C	-0.2359884	-0.9152057	1.6749787
H	3.4304513	-1.0539457	0.3266320
O	2.8839293	-2.8864229	1.9698074
H	0.2372654	-2.7409785	2.7340992
H	-1.2772839	-0.9105281	2.0351930
N	0.1895135	2.2659540	-0.0653128
H	1.0940955	1.7766872	-3.2253331
C	1.3346492	1.3755574	-2.2357727
C	1.5101649	0.2213884	-1.6611739
C	1.7568852	-1.1496442	-2.1513247
C	2.1801818	-3.7175437	-3.2623512
C	3.0246732	-2.6504279	-3.6120825
C	2.8127054	-1.3738298	-3.0662641
C	0.9208420	-2.2337256	-1.7958153
C	1.1257378	-3.5032770	-2.3559522
H	2.3440281	-4.7186166	-3.6948865
H	3.8567578	-2.8102906	-4.3178720
H	3.4747769	-0.5355053	-3.3349262
H	0.0965800	-2.0672438	-1.0839022
H	0.4559344	-4.3353256	-2.0814602
H	-0.3288160	3.1216373	-0.3112567
C	-1.9823949	1.5233350	0.7739732
C	-4.7489168	1.9946365	1.2280657
C	-3.8909273	1.6593259	2.3018371
C	-2.5326718	1.4245519	2.0765794
C	-2.8455695	1.8705045	-0.2867300
C	-4.2146754	2.1003417	-0.0747566
O	-6.0547404	2.1985750	1.5494690
H	-4.3200517	1.5997385	3.3143149
H	-1.8771432	1.1958545	2.9321193
H	-2.4418454	1.9427006	-1.3104591
H	-4.8538629	2.3556583	-0.9324763
C	-6.9667337	2.5488890	0.5205927
H	-7.0386567	1.7516628	-0.2567495
H	-6.6867477	3.5119097	0.0316236
H	-7.9533948	2.6655222	1.0119679
C	2.5211775	-3.9033562	2.8892150
H	1.7176168	-4.5622496	2.4824823
H	2.1870458	-3.4786642	3.8650232

H 3.4352328 -4.5093316 3.0516238

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-296.98	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	18.22	0.22944	YES	YES
9	a	24.31	0.09629	YES	YES
10	a	29.57	0.35562	YES	YES
11	a	32.77	0.12955	YES	YES
12	a	43.30	0.28450	YES	YES
13	a	48.40	1.17254	YES	YES
14	a	52.25	0.33172	YES	YES
15	a	65.12	0.13582	YES	YES
16	a	78.99	0.14413	YES	YES
17	a	85.48	0.13030	YES	YES
18	a	86.69	0.50394	YES	YES
19	a	94.09	0.75043	YES	YES
20	a	99.10	2.62791	YES	YES
21	a	100.03	0.58182	YES	YES
22	a	125.70	0.20917	YES	YES
23	a	143.38	0.32313	YES	YES
24	a	145.97	0.79017	YES	YES
25	a	152.13	1.76887	YES	YES
26	a	177.98	0.13994	YES	YES
27	a	193.14	1.65087	YES	YES
28	a	203.26	3.59753	YES	YES
29	a	208.08	0.83531	YES	YES
30	a	231.47	1.19931	YES	YES
31	a	239.87	1.29797	YES	YES
32	a	244.45	2.03842	YES	YES
33	a	253.73	1.06308	YES	YES
34	a	288.48	1.17820	YES	YES
35	a	306.57	4.12109	YES	YES
36	a	314.39	1.27095	YES	YES
37	a	332.66	0.94044	YES	YES
38	a	355.46	0.48843	YES	YES
39	a	402.18	0.02761	YES	YES
40	a	411.11	4.82695	YES	YES
41	a	412.86	3.42446	YES	YES
42	a	423.23	0.47428	YES	YES
43	a	452.15	0.15110	YES	YES
44	a	459.15	2.51377	YES	YES
45	a	466.24	2.50035	YES	YES
46	a	479.31	5.60076	YES	YES
47	a	491.13	4.47747	YES	YES
48	a	495.62	4.84184	YES	YES
49	a	499.16	4.12463	YES	YES
50	a	512.83	3.08282	YES	YES

TS_{23ej}

SCF Energy (au) BP86/SV(P) -2814.645959297
SCF Energy (au) PBE0/def2-TZVPP -2814.155882277
SCF Energy (au) PBE0/def2-TZVPP -2814.1661111849 (Toluene Correction)
Zero Point Energy (au) 0.4648176
Chemical Potential (kJ mol^{-1}) 1034.42
Dispersion Correction (au) PBE0/def2-TZVPP -0.09273178

xyz coordinates
63

Mn	1.9306911	1.4020002	0.6830458
C	2.1838181	1.7355158	2.4392325
C	3.6641337	0.9860875	0.4910235
C	2.2510348	3.1212471	0.2232937
O	2.4712664	4.2408521	-0.0256646
O	4.7959451	0.7116684	0.3802884
O	2.3372093	1.9384693	3.5758549
C	-0.8818569	0.7680615	1.2417821
C	-2.3576784	0.9247761	1.2413331
C	-0.1766581	-0.4235535	1.6783525
C	1.2250130	-0.4418934	1.3598469
C	2.0102907	-1.5083179	1.8635362
C	1.4349860	-2.5222176	2.6499970
C	0.0410310	-2.5039740	2.9385402
C	-0.7481153	-1.4663571	2.4562785
H	3.0839960	-1.5361476	1.6273815
O	2.1235925	-3.5612119	3.1902086
H	-0.3769380	-3.3106860	3.5600084
H	-1.8189575	-1.4320486	2.7145749
N	-0.0842866	1.7267082	0.8160727
C	0.8260154	1.4855016	-2.5115280
C	1.2304284	2.7687591	-2.9640986
C	0.8216903	3.2503419	-4.2164899
C	-0.0126781	2.4769118	-5.0424273
C	-0.4330863	1.2069388	-4.6039751
C	-0.0216378	0.7153266	-3.3591703
H	1.8769689	3.3893508	-2.3273141
H	1.1563737	4.2473776	-4.5482167
H	-0.3388016	2.8627253	-6.0224091
H	-1.0902393	0.5914373	-5.2412450
H	-0.3540159	-0.2781091	-3.0184706
C	1.2445243	0.9213366	-1.2469878
C	1.4821055	-0.2274950	-0.6770971
C	1.9529371	-1.5431340	-1.1375304
C	-5.1764461	1.2964760	1.1526703
C	-4.5985342	0.0748947	0.7319111
C	-3.2157782	-0.1069035	0.7812849
C	-2.9480030	2.1390221	1.6560944
C	-4.3374039	2.3326881	1.6198692
O	-6.5306659	1.3738259	1.0713401
H	-5.2665135	-0.7177467	0.3601128
H	-2.7833855	-1.0560987	0.4266622
H	-2.3076940	2.9487000	2.0447980
H	-4.7543672	3.2893905	1.9665970
H	-0.5606966	2.5486784	0.4189116
C	3.5214601	-3.6573375	2.9519756
C	-7.1755115	2.5746779	1.4668446
H	4.0669060	-2.7732336	3.3570887
H	3.7460199	-3.7599460	1.8653516
H	3.8590608	-4.5694592	3.4840392
H	-6.9955334	2.8036794	2.5436660
H	-8.2595994	2.4068834	1.3080940

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H    -6.8460474    3.4422745    0.8477132
C     2.8241651   -4.0194464   -2.2026938
C     3.5730824   -2.8515251   -2.4278871
C     3.1401779   -1.6223110   -1.9054453
C     1.2125691   -2.7276841   -0.9091549
C     1.6404862   -3.9514904   -1.4459562
H     3.1613463   -4.9833076   -2.6190666
H     4.5024448   -2.8937399   -3.0201148
H     3.7255107   -0.7070230   -2.0840277
H     0.2858002   -2.6785507   -0.3153716
H     1.0435503   -4.8619399   -1.2700714
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$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-194.57	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	16.41	0.09106	YES	YES
9	a	18.69	0.13939	YES	YES
10	a	24.84	0.06883	YES	YES
11	a	32.84	0.18714	YES	YES
12	a	36.53	0.67747	YES	YES
13	a	43.45	0.75136	YES	YES
14	a	45.03	0.09858	YES	YES
15	a	49.04	0.02101	YES	YES
16	a	57.92	0.23317	YES	YES
17	a	63.05	0.29982	YES	YES
18	a	74.95	0.57612	YES	YES
19	a	76.87	0.04162	YES	YES
20	a	86.54	0.07244	YES	YES
21	a	92.38	0.33303	YES	YES
22	a	98.55	0.34466	YES	YES
23	a	106.72	2.23100	YES	YES
24	a	114.66	0.40203	YES	YES
25	a	124.04	0.64485	YES	YES
26	a	137.05	1.94375	YES	YES
27	a	150.70	1.72182	YES	YES
28	a	160.05	1.53666	YES	YES
29	a	168.98	0.45894	YES	YES
30	a	186.71	1.45702	YES	YES
31	a	189.01	0.60705	YES	YES
32	a	198.14	2.37796	YES	YES
33	a	222.80	0.28299	YES	YES
34	a	230.16	0.23786	YES	YES
35	a	237.45	1.45215	YES	YES
36	a	249.75	1.01148	YES	YES
37	a	253.15	0.14093	YES	YES
38	a	261.15	2.60947	YES	YES
39	a	294.73	4.15721	YES	YES
40	a	323.23	3.05680	YES	YES
41	a	339.69	0.67976	YES	YES
42	a	357.65	4.33796	YES	YES
43	a	374.48	0.60465	YES	YES
44	a	398.95	3.36470	YES	YES
45	a	402.20	0.12622	YES	YES
46	a	405.90	2.63261	YES	YES
47	a	416.83	0.45536	YES	YES
48	a	419.15	2.87869	YES	YES

49	a	435.25	1.41876	YES	YES
50	a	450.38	0.19487	YES	YES

TS_{23fa}

SCF Energy (au) BP86/SV(P) -2391.953906106
SCF Energy (au) PBE0/def2-TZVPP -2391.506807198
SCF Energy (au) PBE0/def2-TZVPP -2391.5145469127 (Toluene Correction)
Zero Point Energy (au) 0.3208594
Chemical Potential (kJ mol^{-1}) 692.48
Dispersion Correction (au) PBE0/def2-TZVPP -0.06636323

xyz coordinates
45

Mn	1.6823049	-0.1540813	0.7119304
C	2.0823667	0.0299876	2.4662496
C	3.3142989	-0.7703630	0.3633362
C	2.2916770	1.5080239	0.3104084
O	2.8051040	2.5272816	0.0645810
O	4.3832846	-1.1888982	0.1417157
O	2.3252325	0.1410141	3.5993230
C	-1.1529180	-0.6715825	1.5897830
C	-0.9430170	1.5831402	0.9670982
C	-2.3147607	1.8220671	1.1899400
C	-3.1142375	0.7522986	1.6168280
C	-2.5383478	-0.5024504	1.8168618
C	-0.4436773	-1.9368414	1.7767137
C	0.8891064	-2.0045914	1.2620044
C	1.6189977	-3.2041245	1.4916431
C	1.0557362	-4.2830285	2.1764479
C	-0.2732070	-4.2137822	2.6538585
C	-1.0127998	-3.0473244	2.4508552
O	-0.0854716	2.5354261	0.5597101
H	-2.7477230	2.8191459	1.0333578
H	-4.1919682	0.9070197	1.7894065
H	-3.1526392	-1.3556750	2.1355549
H	2.6507360	-3.2910846	1.1112435
H	1.6561477	-5.1924837	2.3484406
H	-0.7180477	-5.0658746	3.1926922
H	-2.0376043	-2.9848091	2.8513895
N	-0.3729834	0.3672597	1.1560503
C	0.3526155	0.3818633	-2.3524857
C	0.9943495	1.5649540	-2.8046371
C	0.5520736	2.2219353	-3.9617036
C	-0.5528760	1.7362858	-4.6840251
C	-1.2105295	0.5744263	-4.2394100
C	-0.7656216	-0.0968195	-3.0932606
H	1.8555215	1.9605836	-2.2470897
H	1.0769613	3.1301816	-4.3027952
H	-0.9020385	2.2615575	-5.5884173
H	-2.0800711	0.1837491	-4.7945666
H	-1.2829623	-1.0061058	-2.7462792
C	0.7881228	-0.3593225	-1.1930104
C	0.9329506	-1.5439861	-0.6899098
H	1.0768716	-2.5764308	-1.0226138
C	-0.5505492	3.8496392	0.2821474
H	-1.3018194	3.8476272	-0.5401194
H	0.3453502	4.4159264	-0.0394656
H	-0.9839389	4.3282658	1.1902184

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-228.81	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	19.11	0.00795	YES	YES
9	a	25.55	0.42080	YES	YES
10	a	36.80	0.24743	YES	YES
11	a	50.02	0.01194	YES	YES
12	a	62.78	0.35860	YES	YES
13	a	74.19	1.54238	YES	YES
14	a	88.21	0.46670	YES	YES
15	a	90.75	0.18401	YES	YES
16	a	99.41	1.03121	YES	YES
17	a	106.93	0.10587	YES	YES
18	a	115.06	0.57837	YES	YES
19	a	124.51	0.24267	YES	YES
20	a	130.62	0.61017	YES	YES
21	a	142.11	0.86214	YES	YES
22	a	157.29	0.55479	YES	YES
23	a	184.92	0.19479	YES	YES
24	a	196.86	1.19340	YES	YES
25	a	215.56	1.28885	YES	YES
26	a	219.99	0.16940	YES	YES
27	a	237.14	1.67363	YES	YES
28	a	259.45	0.14314	YES	YES
29	a	289.72	0.20098	YES	YES
30	a	304.37	0.88957	YES	YES
31	a	332.98	0.97419	YES	YES
32	a	351.21	9.54902	YES	YES
33	a	385.30	2.59182	YES	YES
34	a	403.53	0.11870	YES	YES
35	a	406.94	0.93506	YES	YES
36	a	428.32	0.72794	YES	YES
37	a	447.17	1.62589	YES	YES
38	a	452.76	2.13332	YES	YES
39	a	465.85	10.10407	YES	YES
40	a	478.61	2.11244	YES	YES
41	a	492.64	1.85906	YES	YES
42	a	495.93	11.69786	YES	YES
43	a	510.21	5.47025	YES	YES
44	a	522.54	0.68273	YES	YES
45	a	538.58	11.69373	YES	YES
46	a	549.24	15.95716	YES	YES
47	a	551.00	3.74202	YES	YES
48	a	581.07	5.63391	YES	YES
49	a	584.20	14.70772	YES	YES
50	a	609.52	14.07838	YES	YES

TS_{23fa}'

SCF Energy (au) BP86/SV(P) -2391.943845351
SCF Energy (au) PBE0/def2-TZVPP -2391.497946159
SCF Energy (au) PBE0/def2-TZVPP -2391.5061895680 (Toluene Correction)
Zero Point Energy (au) 0.3205041
Chemical Potential (kJ mol^{-1}) 691.29
Dispersion Correction (au) PBE0/def2-TZVPP -0.06768189

xyz coordinates
45

Mn	1.3110392	1.2919826	0.4372025
C	1.4509833	1.6980167	2.1987554
C	3.0228283	0.8213585	0.3786671
C	1.7953893	2.9380234	-0.1248740
O	2.2046709	3.9514035	-0.5338050
O	4.1482855	0.5024836	0.3461756
O	1.5310264	1.9758415	3.3279080
C	-1.5523798	0.5457394	1.0418146
C	-1.4986120	2.7521652	0.2485363
C	-2.9024106	2.8677863	0.3315387
C	-3.6342364	1.7570910	0.7744980
C	-2.9629776	0.5856278	1.1280883
C	-0.7457941	-0.6197127	1.4129148
C	0.6175561	-0.6239367	0.9817123
C	1.4303899	-1.7145122	1.3919974
C	0.9321047	-2.7317726	2.2105416
C	-0.4190106	-2.7209434	2.6216926
C	-1.2508336	-1.6730210	2.2171497
O	-0.7002393	3.7487217	-0.1755946
H	-3.4111534	3.8006983	0.0535798
H	-4.7332901	1.8131157	0.8378185
H	-3.5200531	-0.3020652	1.4585336
H	2.4804194	-1.7603028	1.0605214
H	1.6004942	-3.5474605	2.5338769
H	-0.8132982	-3.5238275	3.2654803
H	-2.2957236	-1.6488616	2.5674539
N	-0.8365671	1.6221262	0.5948643
H	0.7824923	1.3877611	-2.4572689
C	0.8270174	0.8827240	-1.4868665
C	0.7844700	-0.3219684	-1.0065775
C	0.9209701	-1.6842854	-1.5522209
C	1.1695360	-4.2139431	-2.8018412
C	2.1030016	-3.1991099	-3.0733444
C	1.9792576	-1.9436023	-2.4576369
C	-0.0051991	-2.7178798	-1.2778888
C	0.1145770	-3.9666638	-1.9047448
H	1.2648857	-5.1996778	-3.2869415
H	2.9370347	-3.3850051	-3.7704585
H	2.7109546	-1.1462934	-2.6638590
H	-0.8306913	-2.5304744	-0.5734895
H	-0.6238435	-4.7568831	-1.6894224
C	-1.2549939	4.9970395	-0.5660557
H	-1.9479386	4.8831263	-1.4315429
H	-0.3905350	5.6213350	-0.8662557
H	-1.7896031	5.4880350	0.2793667

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-281.82	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	21.96	0.54731	YES	YES
9	a	27.17	0.31688	YES	YES
10	a	39.40	0.07178	YES	YES
11	a	45.13	0.01735	YES	YES
12	a	59.30	0.80359	YES	YES
13	a	73.87	1.42854	YES	YES
14	a	81.25	0.11047	YES	YES
15	a	89.84	0.12936	YES	YES
16	a	91.63	0.10392	YES	YES
17	a	109.10	0.05579	YES	YES
18	a	111.04	1.52700	YES	YES
19	a	129.12	0.58316	YES	YES
20	a	130.00	0.22055	YES	YES
21	a	142.74	0.77459	YES	YES
22	a	160.87	1.01154	YES	YES
23	a	184.29	0.59976	YES	YES
24	a	185.71	2.74327	YES	YES
25	a	209.39	0.21746	YES	YES
26	a	219.24	3.52486	YES	YES
27	a	226.92	2.15658	YES	YES
28	a	261.16	0.23288	YES	YES
29	a	284.51	0.53013	YES	YES
30	a	300.92	1.42087	YES	YES
31	a	315.13	2.22167	YES	YES
32	a	333.70	0.64837	YES	YES
33	a	402.41	0.38858	YES	YES
34	a	403.00	0.12920	YES	YES
35	a	410.69	4.78803	YES	YES
36	a	443.69	3.35847	YES	YES
37	a	457.29	0.26555	YES	YES
38	a	467.58	0.25933	YES	YES
39	a	475.36	3.06914	YES	YES
40	a	479.63	3.18434	YES	YES
41	a	502.35	7.87649	YES	YES
42	a	509.01	11.22374	YES	YES
43	a	510.08	10.04585	YES	YES
44	a	526.74	6.49210	YES	YES
45	a	541.34	9.55862	YES	YES
46	a	548.14	6.24154	YES	YES
47	a	558.45	15.13916	YES	YES
48	a	564.90	6.13221	YES	YES
49	a	581.38	3.49303	YES	YES
50	a	606.71	40.94505	YES	YES

TS_{23ga}

SCF Energy (au) BP86/SV(P) -2508.390483009
SCF Energy (au) PBE0/def2-TZVPP -2507.907823752
SCF Energy (au) PBE0/def2-TZVPP -2507.9156889379 (Toluene Correction)
Zero Point Energy (au) 0.3677427
Chemical Potential (kJ mol^{-1}) 805.67
Dispersion Correction (au) PBE0/def2-TZVPP -0.08080308

xyz coordinates
51

Mn	1.5248441	-0.5845365	0.6397492
C	1.9479276	-0.1680022	2.3451840
C	3.1531787	-1.2378222	0.3611675
C	2.1434209	0.9801826	-0.0458451
O	2.6918521	1.9009823	-0.5073779
O	4.2221227	-1.6797369	0.1922384
O	2.2034064	0.0904312	3.4519353
C	-1.3262728	-1.0784282	1.4637251
C	-1.1652883	1.1729122	0.7906054
C	-2.5693532	1.2931026	0.7780946
C	-3.3670493	0.1875560	1.1054350
C	-2.7381636	-1.0002992	1.4764198
C	-0.5901441	-2.2833859	1.8490622
C	0.7694752	-2.3633513	1.4202424
C	1.5213038	-3.4987701	1.8290059
C	0.9525439	-4.5042281	2.6153884
C	-0.4005685	-4.4235477	3.0150732
C	-1.1636811	-3.3192696	2.6284128
C	-0.3684453	2.4183943	0.5898400
H	-3.0168067	2.2711242	0.5453896
H	-4.4666693	0.2630063	1.0922184
H	-3.3295190	-1.8843629	1.7555811
H	2.5741119	-3.5971104	1.5150369
H	1.5690844	-5.3632896	2.9303901
H	-0.8469301	-5.2157813	3.6375045
H	-2.2094528	-3.2406564	2.9683437
N	-0.5553920	-0.0151934	1.0669763
C	0.1552864	-0.4653066	-2.4658343
C	0.8115630	0.6114667	-3.1182067
C	0.3520392	1.0840650	-4.3563685
C	-0.7830842	0.5178294	-4.9641111
C	-1.4555771	-0.5377193	-4.3206713
C	-0.9942453	-1.0266136	-3.0914358
H	1.6965534	1.0694607	-2.6547579
H	0.8886911	1.9104129	-4.8516946
H	-1.1442849	0.8987999	-5.9335844
H	-2.3490344	-0.9888064	-4.7841610
H	-1.5217427	-1.8530576	-2.5889030
C	0.6129898	-1.0354979	-1.2186079
C	0.7942461	-2.1456615	-0.5795400
H	0.9486033	-3.2104797	-0.7768708
C	0.9675526	4.8921174	0.3197217
C	1.0864307	4.1530671	1.5096814
C	0.4248956	2.9235896	1.6455242
C	-0.4989074	3.1762558	-0.5944436
C	0.1746010	4.4006849	-0.7311774
H	1.4944440	5.8545831	0.2121793
H	1.7004501	4.5366872	2.3410568
H	0.5127752	2.3515817	2.5829314
H	-1.1148258	2.7888184	-1.4221905
H	0.0810448	4.9738029	-1.6683325

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-220.39	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	7.18	0.04481	YES	YES
9	a	25.98	0.14963	YES	YES
10	a	28.35	0.07413	YES	YES
11	a	46.66	0.05710	YES	YES
12	a	59.46	0.24527	YES	YES
13	a	68.02	0.05833	YES	YES
14	a	74.15	0.04441	YES	YES
15	a	75.96	0.56208	YES	YES
16	a	89.54	0.52008	YES	YES
17	a	93.41	0.21133	YES	YES
18	a	104.63	0.29995	YES	YES
19	a	112.39	0.18400	YES	YES
20	a	119.55	0.10028	YES	YES
21	a	126.31	0.36676	YES	YES
22	a	133.97	0.32997	YES	YES
23	a	156.06	0.27131	YES	YES
24	a	162.45	0.56834	YES	YES
25	a	186.04	0.40033	YES	YES
26	a	205.73	0.28924	YES	YES
27	a	217.74	0.64486	YES	YES
28	a	233.91	0.23953	YES	YES
29	a	243.74	1.42955	YES	YES
30	a	292.38	0.46312	YES	YES
31	a	311.96	0.57499	YES	YES
32	a	334.06	0.79096	YES	YES
33	a	352.03	9.28848	YES	YES
34	a	368.04	0.39060	YES	YES
35	a	390.04	4.82528	YES	YES
36	a	401.29	0.38297	YES	YES
37	a	402.85	0.11789	YES	YES
38	a	423.04	1.79015	YES	YES
39	a	442.50	0.64033	YES	YES
40	a	449.25	2.87375	YES	YES
41	a	464.05	9.91506	YES	YES
42	a	470.92	3.87025	YES	YES
43	a	485.37	1.17087	YES	YES
44	a	496.16	4.18584	YES	YES
45	a	496.70	7.06281	YES	YES
46	a	509.12	5.45970	YES	YES
47	a	522.80	0.52314	YES	YES
48	a	544.46	10.99192	YES	YES
49	a	548.38	10.35088	YES	YES
50	a	553.61	7.49606	YES	YES

TS_{23ga}'

SCF Energy (au) BP86/SV(P) -2508.381424342
SCF Energy (au) PBE0/def2-TZVPP -2507.899292682
SCF Energy (au) PBE0/def2-TZVPP -2507.9076218786 (Toluene Correction)
Zero Point Energy (au) 0.3672553
Chemical Potential (kJ mol^{-1}) 806.64
Dispersion Correction (au) PBE0/def2-TZVPP -0.08140660

xyz coordinates
51

Mn	1.2410302	0.5333857	0.2961025
C	1.5263352	1.0929493	1.9927023
C	2.9071938	-0.0668038	0.1951247
C	1.8221134	2.0394922	-0.5207088
O	2.3096189	2.9125814	-1.1210368
O	4.0048967	-0.4683008	0.1367038
O	1.6945615	1.4668466	3.0848500
C	-1.6597261	-0.0149824	0.9417047
C	-1.5364748	2.1990646	0.1567478
C	-2.9411974	2.2625908	0.0498340
C	-3.7179655	1.1449970	0.3851796
C	-3.0711123	0.0031825	0.8574349
C	-0.9090923	-1.1703598	1.4404657
C	0.4594018	-1.2690511	1.0439718
C	1.2150706	-2.3528122	1.5680757
C	0.6562456	-3.2665642	2.4657516
C	-0.7007262	-3.1607172	2.8435114
C	-1.4788625	-2.1225976	2.3227578
C	-0.7715030	3.4558025	-0.0874276
H	-3.4081654	3.2081733	-0.2644633
H	-4.8162981	1.1754567	0.2970408
H	-3.6447395	-0.8918064	1.1399669
H	2.2676031	-2.4767398	1.2651584
H	1.2811689	-4.0761009	2.8790807
H	-1.1414055	-3.8821409	3.5506334
H	-2.5291042	-2.0190188	2.6420475
N	-0.9031486	1.0552181	0.5435537
H	0.4499847	0.4216045	-2.5439982
C	0.5607354	-0.0039046	-1.5418071
C	0.5742943	-1.1626540	-0.9586258
C	0.7256616	-2.5658496	-1.3849620
C	1.0037271	-5.1939512	-2.3999772
C	1.9155938	-4.1931897	-2.7769453
C	1.7767054	-2.8884252	-2.2778509
C	-0.1787191	-3.5841268	-1.0032094
C	-0.0447128	-4.8831180	-1.5151326
H	1.1107196	-6.2183806	-2.7938696
H	2.7439438	-4.4283081	-3.4657565
H	2.4910807	-2.1013343	-2.5668104
H	-0.9984457	-3.3465788	-0.3070807
H	-0.7656718	-5.6628181	-1.2180546
C	0.5151894	5.9401442	-0.4778100
C	0.6249282	5.2747137	0.7554304
C	-0.0111497	4.0399951	0.9510863
C	-0.8937585	4.1414036	-1.3158616
C	-0.2447296	5.3703487	-1.5131783
H	1.0235453	6.9062034	-0.6319847
H	1.2129245	5.7201377	1.5746824
H	0.0709041	3.5264374	1.9220227
H	-1.4872165	3.6944123	-2.1308931
H	-0.3312525	5.8854934	-2.4841767

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-284.04	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	21.83	0.24742	YES	YES
9	a	26.53	0.04054	YES	YES
10	a	27.55	0.22997	YES	YES
11	a	55.52	0.15441	YES	YES
12	a	58.54	0.19895	YES	YES
13	a	61.78	0.23479	YES	YES
14	a	71.79	0.06660	YES	YES
15	a	76.28	0.41529	YES	YES
16	a	83.91	0.31739	YES	YES
17	a	95.67	0.03798	YES	YES
18	a	99.00	0.00329	YES	YES
19	a	107.45	0.22463	YES	YES
20	a	121.83	0.36120	YES	YES
21	a	126.36	0.65725	YES	YES
22	a	137.69	0.31483	YES	YES
23	a	150.00	0.32541	YES	YES
24	a	162.20	1.30034	YES	YES
25	a	188.41	2.47324	YES	YES
26	a	206.75	0.28675	YES	YES
27	a	213.47	0.30054	YES	YES
28	a	219.86	2.90087	YES	YES
29	a	243.29	2.20485	YES	YES
30	a	286.50	0.19870	YES	YES
31	a	310.92	0.22004	YES	YES
32	a	315.82	3.21257	YES	YES
33	a	336.36	0.22768	YES	YES
34	a	363.76	0.87637	YES	YES
35	a	400.50	0.19138	YES	YES
36	a	403.33	0.02312	YES	YES
37	a	410.28	4.24302	YES	YES
38	a	428.24	3.94233	YES	YES
39	a	452.97	0.04614	YES	YES
40	a	463.34	1.26011	YES	YES
41	a	471.28	2.93625	YES	YES
42	a	476.39	2.12371	YES	YES
43	a	491.14	1.06595	YES	YES
44	a	499.32	3.23268	YES	YES
45	a	509.11	20.73100	YES	YES
46	a	511.47	2.04412	YES	YES
47	a	527.22	1.86051	YES	YES
48	a	542.20	12.79466	YES	YES
49	a	553.78	5.71313	YES	YES
50	a	559.95	14.88453	YES	YES

TS_{23ha}

SCF Energy (au) BP86/SV(P) -2354.862307833
SCF Energy (au) PBE0/def2-TZVPP -2354.406354751
SCF Energy (au) PBE0/def2-TZVPP -2354.4142715193 (Toluene Correction)
Zero Point Energy (au) 0.3226651
Chemical Potential (kJ mol^{-1}) 696.08
Dispersion Correction (au) PBE0/def2-TZVPP -0.06451629

xyz coordinates
45

Mn	2.2084975	0.5250623	0.5478324
C	2.6176997	0.7441853	2.2909833
C	3.9129016	0.0878398	0.1836519
C	2.5072647	2.2676112	0.1533830
O	2.7042883	3.3973215	-0.0618477
O	5.0195021	-0.2048262	-0.0461420
O	2.8692686	0.8708948	3.4207629
C	-0.5551355	-0.0946769	1.2974896
C	-2.0218377	0.1023037	1.4525877
C	0.1473763	-1.3403631	1.5748185
C	1.5219795	-1.3471266	1.1580807
C	2.2933222	-2.4938345	1.4860373
C	1.7320956	-3.5737157	2.1751747
C	0.3709319	-3.5602620	2.5605212
C	-0.4165103	-2.4465547	2.2606540
H	3.3550933	-2.5382253	1.1887155
H	2.3632348	-4.4427922	2.4280768
H	-0.0603429	-4.4147024	3.1066682
H	-1.4689279	-2.4092071	2.5857970
N	0.2270115	0.8730877	0.8742984
C	0.9202487	0.8497547	-2.5944228
C	1.4599919	2.0800371	-3.0524654
C	0.9950442	2.6676223	-4.2376942
C	-0.0284697	2.0583820	-4.9852224
C	-0.5822600	0.8444312	-4.5379431
C	-0.1163384	0.2449687	-3.3610110
H	2.2572838	2.5714496	-2.4764361
H	1.4363998	3.6186356	-4.5793264
H	-0.3965910	2.5289268	-5.9117454
H	-1.3869890	0.3575539	-5.1140262
H	-0.5514575	-0.7048071	-3.0108143
C	1.3904782	0.1728235	-1.4093728
C	1.6563040	-0.9615126	-0.8514462
H	1.9301743	-1.9875303	-1.1118527
C	-4.8044947	0.5537602	1.6782051
C	-4.3265595	-0.6013673	1.0345916
C	-2.9461264	-0.8304895	0.9262954
C	-2.5138801	1.2629604	2.0949284
C	-3.8947102	1.4844429	2.2095130
H	-5.8894386	0.7282725	1.7672252
H	-5.0359508	-1.3295173	0.6079751
H	-2.5756396	-1.7276806	0.4049310
H	-1.8032385	1.9844021	2.5317119
H	-4.2629510	2.3874861	2.7235363
H	-0.2585430	1.7449751	0.6173225

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-211.06	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	18.67	0.09950	YES	YES
9	a	21.60	0.02891	YES	YES
10	a	38.38	0.00779	YES	YES
11	a	48.05	0.09372	YES	YES
12	a	51.86	0.11616	YES	YES
13	a	69.55	0.22643	YES	YES
14	a	73.33	0.08989	YES	YES
15	a	80.49	0.12999	YES	YES
16	a	88.89	0.07702	YES	YES
17	a	94.68	0.23259	YES	YES
18	a	103.22	0.02377	YES	YES
19	a	110.35	0.25271	YES	YES
20	a	134.35	0.18439	YES	YES
21	a	143.04	0.44549	YES	YES
22	a	176.35	0.76100	YES	YES
23	a	195.95	0.47683	YES	YES
24	a	204.67	0.63859	YES	YES
25	a	212.39	0.45590	YES	YES
26	a	238.72	0.78590	YES	YES
27	a	269.37	1.77691	YES	YES
28	a	304.64	0.65671	YES	YES
29	a	340.16	8.47923	YES	YES
30	a	358.93	0.43972	YES	YES
31	a	395.36	1.89545	YES	YES
32	a	402.38	0.02315	YES	YES
33	a	404.64	0.38999	YES	YES
34	a	420.53	1.91042	YES	YES
35	a	436.65	0.58360	YES	YES
36	a	447.96	4.00709	YES	YES
37	a	461.40	20.24491	YES	YES
38	a	465.05	2.25747	YES	YES
39	a	485.47	0.85113	YES	YES
40	a	492.96	2.86485	YES	YES
41	a	497.08	3.33844	YES	YES
42	a	504.77	8.24943	YES	YES
43	a	521.80	0.45494	YES	YES
44	a	540.22	19.26739	YES	YES
45	a	544.86	15.56428	YES	YES
46	a	564.68	28.71926	YES	YES
47	a	590.89	1.48234	YES	YES
48	a	609.57	1.75365	YES	YES
49	a	611.76	5.86176	YES	YES
50	a	618.68	13.41133	YES	YES

TS_{23ia}

SCF Energy (au) BP86/SV(P) -2183.113967934
SCF Energy (au) PBE0/def2-TZVPP -2182.694332982
SCF Energy (au) PBE0/def2-TZVPP -2182.7012637601 (Toluene Correction)
Zero Point Energy (au) 0.2578498
Chemical Potential (kJ mol^{-1}) 537.65
Dispersion Correction (au) PBE0/def2-TZVPP -0.05000930

xyz coordinates
37

Mn	1.3012750	0.6735212	0.8636467
C	1.6923990	0.9350102	2.6106761
C	3.0056460	0.2982574	0.5195438
C	1.5195873	2.4381721	0.4701240
O	1.6680679	3.5695831	0.2467560
O	4.1188443	0.0253376	0.2925176
O	1.9402074	1.0881191	3.7374012
C	-1.4133247	0.0725285	1.6759428
C	-2.8893810	0.2622864	1.9251222
C	-0.7120733	-1.1720529	1.9402837
C	0.6484269	-1.1933217	1.4760537
C	1.4170669	-2.3495710	1.7900079
C	0.8606475	-3.4172984	2.4976908
C	-0.4970965	-3.3998829	2.9059424
C	-1.2792418	-2.2813597	2.6211696
H	2.4683728	-2.4084477	1.4609439
H	1.4898509	-4.2905435	2.7409042
H	-0.9242473	-4.2576205	3.4497033
H	-2.3326827	-2.2471590	2.9453367
O	-0.7429383	1.0326985	1.2089872
C	0.1325468	0.9718078	-2.2911245
C	0.7714301	2.1345748	-2.7930459
C	0.3824316	2.6896191	-4.0202216
C	-0.6628773	2.1152407	-4.7650935
C	-1.3143103	0.9685711	-4.2745778
C	-0.9219310	0.3997316	-3.0562753
H	1.5860925	2.5985052	-2.2181170
H	0.8988533	3.5882855	-4.3963692
H	-0.9726876	2.5619450	-5.7242020
H	-2.1370795	0.5107462	-4.8488892
H	-1.4327901	-0.4979350	-2.6718159
C	0.5245875	0.3310298	-1.0565555
C	0.7064571	-0.8183133	-0.4815302
H	0.9010254	-1.8573590	-0.7651214
H	-3.1924575	1.2771447	1.5999085
H	-3.1200868	0.1456830	3.0077219
H	-3.4886102	-0.4975339	1.3765547

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-228.38	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	18.98	0.12008	YES	YES
9	a	28.24	0.16870	YES	YES
10	a	56.30	0.07960	YES	YES

11	a	57.56	0.36639	YES	YES
12	a	73.76	0.43554	YES	YES
13	a	77.76	0.29842	YES	YES
14	a	90.84	0.23664	YES	YES
15	a	98.00	0.44156	YES	YES
16	a	103.22	0.33827	YES	YES
17	a	109.70	0.29581	YES	YES
18	a	123.22	0.04442	YES	YES
19	a	139.00	0.13164	YES	YES
20	a	160.46	0.60555	YES	YES
21	a	183.73	0.72674	YES	YES
22	a	202.28	0.19418	YES	YES
23	a	217.24	1.59049	YES	YES
24	a	246.57	1.24502	YES	YES
25	a	268.54	0.12494	YES	YES
26	a	284.53	0.22753	YES	YES
27	a	344.37	6.19449	YES	YES
28	a	378.18	1.40902	YES	YES
29	a	401.89	0.07019	YES	YES
30	a	410.53	2.74233	YES	YES
31	a	412.51	0.38710	YES	YES
32	a	437.47	1.28361	YES	YES
33	a	451.81	0.33644	YES	YES
34	a	461.91	10.89574	YES	YES
35	a	474.64	1.21843	YES	YES
36	a	489.37	4.15812	YES	YES
37	a	499.02	12.59916	YES	YES
38	a	507.71	2.91113	YES	YES
39	a	523.72	0.68396	YES	YES
40	a	536.45	21.31995	YES	YES
41	a	544.19	10.51342	YES	YES
42	a	587.29	45.28376	YES	YES
43	a	601.55	8.05846	YES	YES
44	a	605.21	3.61664	YES	YES
45	a	610.37	16.40323	YES	YES
46	a	618.62	32.05822	YES	YES
47	a	629.66	5.92647	YES	YES
48	a	650.99	6.48357	YES	YES
49	a	662.64	77.38872	YES	YES
50	a	683.14	75.60527	YES	YES

TS_{23ia}'

SCF Energy (au) BP86/SV(P) -2183.103988116
SCF Energy (au) PBE0/def2-TZVPP -2182.684894240
SCF Energy (au) PBE0/def2-TZVPP -2182.6918100274 (Toluene Correction)
Zero Point Energy (au) 0.2574986
Chemical Potential (kJ mol^{-1}) 536.55
Dispersion Correction (au) PBE0/def2-TZVPP -0.05277314

xyz coordinates
37

Mn	0.8656508	2.1918527	0.3154680
C	1.1790350	2.5549686	2.0654266
C	2.5879855	1.8447707	0.0639702
C	1.0592617	3.9108963	-0.2271348
O	1.1764375	5.0000906	-0.6170753
O	3.7169389	1.5924075	-0.1107837
O	1.3780395	2.7885345	3.1888876
C	-1.8851770	1.5606129	1.0314934
C	-3.3749241	1.7211766	1.2143033
C	-1.1676374	0.3385116	1.3637880
C	0.1928795	0.2976471	0.8966920
C	0.9769784	-0.8171162	1.3068905
C	0.4509880	-1.8082698	2.1384112
C	-0.9031338	-1.7728671	2.5530957
C	-1.7117010	-0.7081467	2.1532768
H	2.0212614	-0.8984200	0.9639711
H	1.0995558	-2.6375996	2.4677812
H	-1.3097820	-2.5737732	3.1913226
H	-2.7632831	-0.6596729	2.4818752
O	-1.2156307	2.5215978	0.5717577
H	0.0508076	2.2612256	-2.5157530
C	0.2007315	1.7823629	-1.5430835
C	0.2860068	0.5846236	-1.0359600
C	0.5162019	-0.7600306	-1.6056033
H	-3.6912993	2.7092654	0.8251728
H	-3.6424525	1.6592183	2.2930281
H	-3.9340442	0.9161822	0.6885007
C	0.9322564	-3.2571365	-2.8686490
C	1.8416603	-2.2050001	-3.0704459
C	1.6339749	-0.9629319	-2.4495997
C	-0.3846345	-1.8296872	-1.3973801
C	-0.1825077	-3.0636265	-2.0332442
H	1.0923530	-4.2302003	-3.3619071
H	2.7212031	-2.3489816	-3.7198076
H	2.3454830	-0.1362331	-2.6045609
H	-1.2567891	-1.6828597	-0.7402380
H	-0.9026940	-3.8833917	-1.8738868

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-289.58	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	19.52	0.07940	YES	YES
9	a	29.50	0.44592	YES	YES
10	a	47.00	0.00881	YES	YES

11	a	66.99	0.70250	YES	YES
12	a	69.94	0.36195	YES	YES
13	a	75.16	0.35748	YES	YES
14	a	87.37	0.16474	YES	YES
15	a	92.36	0.09761	YES	YES
16	a	100.95	0.18832	YES	YES
17	a	105.08	0.60387	YES	YES
18	a	125.50	0.05780	YES	YES
19	a	145.83	0.68043	YES	YES
20	a	161.43	0.37167	YES	YES
21	a	189.20	2.75605	YES	YES
22	a	201.91	1.88209	YES	YES
23	a	214.20	1.99503	YES	YES
24	a	233.76	2.14063	YES	YES
25	a	247.68	0.55556	YES	YES
26	a	280.54	0.32179	YES	YES
27	a	305.53	1.16879	YES	YES
28	a	391.57	2.59632	YES	YES
29	a	400.96	0.00811	YES	YES
30	a	409.44	2.07552	YES	YES
31	a	418.83	5.94734	YES	YES
32	a	445.08	0.94194	YES	YES
33	a	466.52	0.52551	YES	YES
34	a	474.78	0.62650	YES	YES
35	a	486.70	3.71712	YES	YES
36	a	497.96	17.15639	YES	YES
37	a	510.90	0.65377	YES	YES
38	a	514.70	9.50928	YES	YES
39	a	523.80	7.85160	YES	YES
40	a	535.03	12.63137	YES	YES
41	a	562.79	13.26407	YES	YES
42	a	569.97	6.56249	YES	YES
43	a	599.46	22.92425	YES	YES
44	a	604.08	9.15845	YES	YES
45	a	610.41	63.96900	YES	YES
46	a	613.73	5.51951	YES	YES
47	a	628.85	10.60410	YES	YES
48	a	656.49	38.14813	YES	YES
49	a	681.82	76.06539	YES	YES
50	a	689.44	19.04587	YES	YES

TS_{23ja}

SCF Energy (au) BP86/SV(P) -2452.074142234
SCF Energy (au) PBE0/def2-TZVPP -2451.611763009
SCF Energy (au) PBE0/def2-TZVPP -2451.6198030278 (Toluene Correction)
Zero Point Energy (au) 0.3426121
Chemical Potential (kJ mol^{-1}) 738.90
Dispersion Correction (au) PBE0/def2-TZVPP -0.06697983

xyz coordinates
48

Mn	1.5654786	0.9681938	0.4627900
C	1.9182416	1.2711050	2.2078398
C	3.2854914	0.6398468	0.1205255
C	1.7410987	2.7390327	0.0539965
O	1.8481311	3.8736680	-0.1726503
O	4.4094621	0.4308376	-0.1165767
O	2.1443005	1.4632721	3.3334955
C	-1.1354830	0.3230288	1.1767272
C	-2.5924500	0.4860401	1.4246771
C	-0.4263610	-0.8978221	1.4068286
C	0.9262225	-0.8932344	1.0551879
C	1.7359861	-2.1102219	1.3285877
O	-0.4687028	1.3262799	0.7545599
C	0.4294030	1.3443794	-2.7203335
C	1.0947815	2.4917352	-3.2222126
C	0.6939823	3.0742199	-4.4328112
C	-0.3837235	2.5396352	-5.1609371
C	-1.0597128	1.4079526	-4.6693880
C	-0.6607253	0.8148338	-3.4650582
H	1.9398299	2.9201504	-2.6636380
H	1.2293198	3.9607478	-4.8111972
H	-0.6992564	3.0056133	-6.1089827
H	-1.9080140	0.9816840	-5.2305998
H	-1.1914557	-0.0692529	-3.0769267
C	0.8343937	0.6607428	-1.5140208
C	1.0386082	-0.4801990	-0.9434658
H	1.2698459	-1.5240326	-1.1830719
C	3.2211616	-4.4623286	1.9036248
C	1.9746975	-4.5548126	1.2605153
C	1.2370539	-3.3932483	0.9855944
C	3.0006889	-2.0360127	1.9592241
C	3.7266886	-3.1994438	2.2567531
H	3.8001881	-5.3739688	2.1256541
H	1.5719437	-5.5398198	0.9715006
H	0.2581377	-3.4736495	0.4834480
H	3.4100301	-1.0544150	2.2403214
H	4.7022422	-3.1159529	2.7634979
C	-5.3471196	0.8537170	1.9156071
C	-4.8631252	-0.4103499	1.5360898
C	-3.4918806	-0.5979408	1.3053365
C	-3.0919689	1.7596975	1.7845470
C	-4.4577647	1.9373832	2.0431648
H	-6.4229519	0.9971777	2.1104698
H	-5.5601838	-1.2565457	1.4170325
H	-3.1189453	-1.5882096	0.9971250
H	-2.3856525	2.5997060	1.8729524
H	-4.8346486	2.9278332	2.3479318
H	-0.9072833	-1.7670527	1.8862643

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-180.13	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	16.16	0.08999	YES	YES
9	a	20.23	0.17454	YES	YES
10	a	34.71	0.06401	YES	YES
11	a	37.61	0.19479	YES	YES
12	a	43.85	0.24760	YES	YES
13	a	51.29	0.13596	YES	YES
14	a	54.50	0.27276	YES	YES
15	a	63.64	0.23335	YES	YES
16	a	74.41	0.09767	YES	YES
17	a	93.89	0.26720	YES	YES
18	a	99.92	0.26287	YES	YES
19	a	102.96	0.22256	YES	YES
20	a	105.64	0.21123	YES	YES
21	a	116.39	0.20491	YES	YES
22	a	143.20	0.60293	YES	YES
23	a	149.93	0.16503	YES	YES
24	a	190.48	1.23144	YES	YES
25	a	205.11	1.14525	YES	YES
26	a	214.53	0.46048	YES	YES
27	a	220.33	0.23064	YES	YES
28	a	237.52	0.32706	YES	YES
29	a	247.55	0.52677	YES	YES
30	a	282.57	2.82391	YES	YES
31	a	341.14	1.83436	YES	YES
32	a	353.75	3.35426	YES	YES
33	a	366.36	8.42762	YES	YES
34	a	401.05	0.75597	YES	YES
35	a	401.37	0.17593	YES	YES
36	a	404.09	1.14187	YES	YES
37	a	421.75	0.55163	YES	YES
38	a	438.05	4.88263	YES	YES
39	a	445.64	5.18937	YES	YES
40	a	467.10	3.82912	YES	YES
41	a	469.55	9.05303	YES	YES
42	a	492.57	4.87405	YES	YES
43	a	495.94	4.92155	YES	YES
44	a	498.59	9.00082	YES	YES
45	a	516.90	5.21897	YES	YES
46	a	522.34	2.90990	YES	YES
47	a	539.29	7.89970	YES	YES
48	a	550.81	20.25726	YES	YES
49	a	556.18	47.74073	YES	YES
50	a	584.71	36.46291	YES	YES

TS_{38ia}

SCF Energy (au) BP86/SV(P) -2183.131539912
SCF Energy (au) PBE0/def2-TZVPP -2182.721878063
SCF Energy (au) PBE0/def2-TZVPP -2182.7291178777 (Toluene Correction)
Zero Point Energy (au) 0.2598847
Chemical Potential (kJ mol^{-1}) 548.92
Dispersion Correction (au) PBE0/def2-TZVPP -0.05353197

xyz coordinates
37

C	1.3367351	-0.3768756	2.2988397
C	-0.8696697	0.8718326	2.5792574
C	0.2856535	0.5555105	-0.1853000
C	-0.8282425	-1.6478829	2.9806592
C	1.2519233	-1.5778408	-0.5630382
C	2.2661993	-2.5523916	-0.6927707
C	0.7030816	-4.2683414	0.1152815
C	-0.3271217	-3.3227472	0.2125609
C	-0.0654066	-1.9849484	-0.1596621
C	-1.1360361	-0.9068470	-0.3388982
C	-1.5758540	-0.6336499	-1.7822888
Mn	-0.3279993	-0.5396906	1.6508554
O	-2.0534784	-0.8175555	0.5732889
O	2.4163054	-0.2735892	2.7286415
O	-1.2253325	1.7938260	3.1976814
C	1.3383776	-0.1411305	-0.7477564
O	-1.1596605	-2.3668982	3.8350984
C	1.9817374	-3.8823686	-0.3520192
H	2.1689385	0.3057951	-1.3249510
C	-0.0172476	1.9784906	-0.3980815
C	-0.6588862	4.7126596	-0.8344551
C	-1.6449917	3.8175246	-0.3849215
C	-1.3271176	2.4705144	-0.1582523
C	0.9650262	2.8969337	-0.8540831
C	0.6494950	4.2465958	-1.0614716
H	-0.9056341	5.7744510	-0.9996448
H	-2.6712222	4.1733747	-0.1962435
H	-2.1011877	1.7750955	0.2048468
H	1.9976462	2.5529194	-1.0266605
H	1.4329602	4.9443609	-1.4014742
H	-1.3413772	-3.6078647	0.5360664
H	0.5161972	-5.3184823	0.3920617
H	2.7777451	-4.6417863	-0.4299211
H	3.2777694	-2.2619577	-1.0205504
H	-0.7404145	-0.7332922	-2.5036776
H	-2.0291270	0.3746046	-1.8699356
H	-2.3597839	-1.3883484	-2.0190815

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-178.15	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	38.07	0.17468	YES	YES
9	a	42.16	0.34856	YES	YES
10	a	57.65	0.64808	YES	YES
11	a	69.07	0.05984	YES	YES

12	a	79.69	1.20659	YES	YES
13	a	85.09	0.07459	YES	YES
14	a	91.20	0.11329	YES	YES
15	a	101.05	0.11238	YES	YES
16	a	108.83	0.07859	YES	YES
17	a	109.28	0.33871	YES	YES
18	a	129.11	1.29873	YES	YES
19	a	172.76	1.55207	YES	YES
20	a	197.82	1.60561	YES	YES
21	a	218.20	1.84289	YES	YES
22	a	229.25	1.86660	YES	YES
23	a	250.83	0.90614	YES	YES
24	a	261.45	5.14381	YES	YES
25	a	277.68	0.84444	YES	YES
26	a	299.35	0.12607	YES	YES
27	a	346.64	4.71924	YES	YES
28	a	365.64	21.12433	YES	YES
29	a	405.32	0.81981	YES	YES
30	a	442.72	2.88639	YES	YES
31	a	448.97	1.12164	YES	YES
32	a	463.59	3.13786	YES	YES
33	a	472.79	2.09847	YES	YES
34	a	486.71	13.64170	YES	YES
35	a	489.97	4.34087	YES	YES
36	a	498.19	5.76372	YES	YES
37	a	518.61	14.10605	YES	YES
38	a	526.22	1.99394	YES	YES
39	a	532.54	1.56273	YES	YES
40	a	538.83	2.68195	YES	YES
41	a	545.65	5.39873	YES	YES
42	a	578.06	50.23447	YES	YES
43	a	605.11	1.59629	YES	YES
44	a	612.32	2.01782	YES	YES
45	a	625.64	19.88850	YES	YES
46	a	631.86	24.17884	YES	YES
47	a	640.70	6.88353	YES	YES
48	a	687.72	43.96053	YES	YES
49	a	697.76	24.66806	YES	YES
50	a	707.48	1.42323	YES	YES

TS_{38ja}

SCF Energy (au) BP86/SV(P) -2452.085970536
SCF Energy (au) PBE0/def2-TZVPP -2451.630064256
SCF Energy (au) PBE0/def2-TZVPP -2451.6393433949 (Toluene Correction)
Zero Point Energy (au) 0.3438944
Chemical Potential (kJ mol^{-1}) 742.05
Dispersion Correction (au) PBE0/def2-TZVPP -0.07029183

xyz coordinates
48

C	1.4459651	-0.1758419	2.8322908
C	-0.8719835	0.8033845	3.3521899
C	0.0125768	0.8884238	0.4443620
C	-0.5083544	-1.7779318	3.3370157
C	1.0132788	-1.2451803	0.1905398
C	2.1795258	-2.1580859	0.1205537
C	-0.3067939	-1.6681079	0.4295187
C	-1.4034456	-0.6318798	0.2980345
C	-2.0187606	-0.3064184	-1.0455662
Mn	-0.2219443	-0.4141605	2.2012076
O	-2.1573556	-0.5843903	1.3513091
O	2.5026577	-0.0181497	3.3015286
O	-1.3089156	1.5830339	4.0958950
C	1.0950577	0.1951911	-0.0519171
O	-0.7006179	-2.6852305	4.0434619
H	1.9811696	0.6399284	-0.5426852
C	-0.2991287	2.3090379	0.2745308
C	-0.9605832	5.0546709	-0.0279566
C	-1.8643864	4.1740186	0.5920341
C	-1.5362569	2.8195546	0.7454660
C	0.5953798	3.2118961	-0.3598140
C	0.2720649	4.5675809	-0.5018172
H	-1.2138114	6.1218979	-0.1407718
H	-2.8323003	4.5476008	0.9648278
H	-2.2417561	2.1306412	1.2353915
H	1.5655869	2.8492619	-0.7365969
H	0.9880235	5.2532203	-0.9851804
C	4.3876931	-3.9295352	-0.0631820
C	4.4216323	-2.6878733	-0.7187161
C	3.3334881	-1.8068533	-0.6202468
C	2.1615645	-3.4136922	0.7770749
C	3.2539196	-4.2864338	0.6895042
H	5.2462816	-4.6173137	-0.1331958
H	5.3049295	-2.3975818	-1.3107729
H	3.3789063	-0.8420686	-1.1485920
H	1.2920379	-3.6977317	1.3904486
H	3.2228163	-5.2524159	1.2194816
C	-3.3354897	0.2099527	-3.4882376
C	-2.0171691	-0.2836324	-3.4855670
C	-1.3643536	-0.5440095	-2.2721703
C	-3.3403718	0.1856946	-1.0537263
C	-3.9954496	0.4391063	-2.2694879
H	-3.8483526	0.4108975	-4.4436166
H	-1.4963679	-0.4734897	-4.4387979
H	-0.3342230	-0.9371152	-2.2802273
H	-3.8489404	0.3411595	-0.0895448
H	-5.0318163	0.8173070	-2.2638959
H	-0.5956271	-2.7183371	0.5856160

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-257.50	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	16.16	0.35618	YES	YES
9	a	19.51	0.10998	YES	YES
10	a	30.74	0.85372	YES	YES
11	a	37.52	0.01350	YES	YES
12	a	40.58	0.13918	YES	YES
13	a	47.33	0.01430	YES	YES
14	a	51.11	0.28303	YES	YES
15	a	59.59	0.80674	YES	YES
16	a	74.06	0.79660	YES	YES
17	a	84.46	0.71821	YES	YES
18	a	89.28	0.09853	YES	YES
19	a	100.80	0.74385	YES	YES
20	a	110.29	1.42942	YES	YES
21	a	124.54	0.19616	YES	YES
22	a	133.27	0.44369	YES	YES
23	a	157.79	2.33843	YES	YES
24	a	187.55	0.58258	YES	YES
25	a	203.50	1.02218	YES	YES
26	a	218.94	3.89951	YES	YES
27	a	235.58	1.10036	YES	YES
28	a	242.37	0.84239	YES	YES
29	a	249.53	0.58950	YES	YES
30	a	290.62	8.45380	YES	YES
31	a	355.98	18.12758	YES	YES
32	a	373.78	1.88651	YES	YES
33	a	396.89	1.42140	YES	YES
34	a	400.74	0.64740	YES	YES
35	a	402.24	0.55560	YES	YES
36	a	416.32	11.16342	YES	YES
37	a	438.96	1.67739	YES	YES
38	a	456.34	7.67132	YES	YES
39	a	462.49	3.16918	YES	YES
40	a	473.97	8.00078	YES	YES
41	a	478.28	0.19856	YES	YES
42	a	480.96	1.70836	YES	YES
43	a	494.62	8.40481	YES	YES
44	a	507.88	11.33733	YES	YES
45	a	517.95	4.88110	YES	YES
46	a	528.96	16.19087	YES	YES
47	a	541.68	2.52103	YES	YES
48	a	576.51	14.87999	YES	YES
49	a	588.03	27.43969	YES	YES
50	a	607.72	15.80706	YES	YES

TS_{39ia}

SCF Energy (au) BP86/SV(P) -2183.125430263
SCF Energy (au) PBE0/def2-TZVPP -2182.704202665
SCF Energy (au) PBE0/def2-TZVPP -2182.7106225495 (Toluene Correction)
Zero Point Energy (au) 0.2592413
Chemical Potential (kJ mol^{-1}) 544.22
Dispersion Correction (au) PBE0/def2-TZVPP -0.04988049

xyz coordinates

37			
C	1.6215828	0.0130222	2.8637253
C	-0.5552919	1.2926508	2.8384885
C	0.3174606	0.8443706	0.1505579
C	-0.5744828	-1.3750881	3.0075668
C	0.7261198	-1.6256458	0.3393932
C	1.7321269	-2.6532331	0.5664832
C	0.2907708	-4.3516046	-0.4519661
C	-0.7080140	-3.4292694	-0.6772707
C	-0.5704676	-2.0679884	-0.2341211
C	-1.5464973	-1.0762966	-0.3232095
C	-2.7473448	-1.0344039	-1.2212595
Mn	0.1193950	-0.0917515	1.9197951
O	-1.3230132	0.0275928	0.4074424
O	2.6326727	0.0755906	3.4481464
O	-0.9747757	2.1891404	3.4576197
C	1.1731735	-0.2558642	0.0899197
O	-1.0479384	-2.1858525	3.6955779
C	1.5161086	-3.9592029	0.1995257
H	2.2538640	-0.0815612	-0.0572638
C	0.3137643	2.1154790	-0.5445059
H	-1.6541747	-3.7437835	-1.1471547
H	0.1515968	-5.4016114	-0.7567116
H	2.2932074	-4.7178198	0.3894030
H	2.6884546	-2.3521242	1.0258805
H	-2.8894473	-1.9851829	-1.7739075
H	-2.6294363	-0.2159190	-1.9692374
H	-3.6716583	-0.8108671	-0.6431154
C	0.3086756	4.5642397	-1.9674185
C	0.8512904	3.4089457	-2.5600222
C	0.8486286	2.1954004	-1.8602233
C	-0.2351322	3.2887501	0.0356064
C	-0.2339798	4.4983769	-0.6702443
H	0.3059966	5.5188076	-2.5194580
H	1.2749335	3.4550747	-3.5766716
H	1.2615609	1.2851469	-2.3259539
H	-0.6594449	3.2401770	1.0493161
H	-0.6602843	5.4023044	-0.2047327

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-313.32	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	31.63	0.03949	YES	YES
9	a	40.30	0.01775	YES	YES
10	a	53.45	0.53751	YES	YES
11	a	60.98	0.12144	YES	YES
12	a	69.36	0.04757	YES	YES

13	a	80.92	0.16401	YES	YES
14	a	88.84	0.18539	YES	YES
15	a	91.39	0.29083	YES	YES
16	a	98.17	0.47781	YES	YES
17	a	104.25	0.53446	YES	YES
18	a	122.27	0.27990	YES	YES
19	a	147.04	0.95015	YES	YES
20	a	154.86	1.55796	YES	YES
21	a	192.89	0.67278	YES	YES
22	a	223.70	0.31201	YES	YES
23	a	235.13	0.54397	YES	YES
24	a	257.58	0.44732	YES	YES
25	a	279.00	0.69986	YES	YES
26	a	318.53	1.92914	YES	YES
27	a	387.67	4.46802	YES	YES
28	a	403.37	0.08995	YES	YES
29	a	417.51	2.41069	YES	YES
30	a	432.74	1.95993	YES	YES
31	a	441.60	2.11914	YES	YES
32	a	461.74	0.87129	YES	YES
33	a	477.70	3.83105	YES	YES
34	a	478.89	0.99679	YES	YES
35	a	482.93	1.29028	YES	YES
36	a	501.38	0.56334	YES	YES
37	a	510.65	3.16652	YES	YES
38	a	520.78	7.08188	YES	YES
39	a	535.43	14.46453	YES	YES
40	a	542.00	5.87021	YES	YES
41	a	566.54	4.99136	YES	YES
42	a	581.36	9.04895	YES	YES
43	a	603.70	18.18185	YES	YES
44	a	614.09	33.72873	YES	YES
45	a	631.46	6.20273	YES	YES
46	a	642.41	31.94297	YES	YES
47	a	657.03	5.78668	YES	YES
48	a	685.30	47.75021	YES	YES
49	a	688.80	33.16830	YES	YES
50	a	701.59	14.32620	YES	YES

TS_{39ja}

SCF Energy (au) BP86/SV(P) -2452.101612798
SCF Energy (au) PBE0/def2-TZVPP -2451.637427819
SCF Energy (au) PBE0/def2-TZVPP -2451.6455080397 (Toluene Correction)
Zero Point Energy (au) 0.3446137
Chemical Potential (kJ mol^{-1}) 746.48
Dispersion Correction (au) PBE0/def2-TZVPP -0.06671155

xyz coordinates
48

C	1.6911518	0.6228639	2.9599087
C	-0.5381033	1.8319302	2.8699088
C	0.5156193	1.3664366	0.2758119
C	-0.4804033	-0.7971369	3.1531878
C	0.8488824	-1.1533185	0.4898860
C	1.9238833	-2.1593889	0.7807363
C	-0.4299699	-1.6306059	-0.0101577
C	-1.4614591	-0.7019179	-0.1204781
C	-2.6568288	-0.7785329	-0.9969108
Mn	0.1931996	0.4441162	2.0089345
O	-1.3093976	0.4176004	0.5715432
O	2.6893899	0.7487136	3.5529774
O	-1.0018127	2.7373071	3.4424823
C	1.2831257	0.2088211	0.1935954
O	-0.9329596	-1.5831127	3.8847944
H	2.3746248	0.3488222	0.0759198
C	0.5527362	2.6114123	-0.4457787
C	-4.9714533	-0.8042816	-2.6347098
C	-4.0882095	-1.8996863	-2.6367533
C	-2.9367838	-1.8859868	-1.8347872
C	-3.5595053	0.3131106	-0.9985137
C	-4.6981174	0.3043616	-1.8148038
H	-5.8716749	-0.8147227	-3.2716781
H	-4.2965941	-2.7715272	-3.2790539
H	-2.2505973	-2.7475411	-1.8679982
H	-3.3418301	1.1706181	-0.3448872
H	-5.3818132	1.1696513	-1.8054271
H	-0.4897308	-2.6480544	-0.4272459
C	0.6920922	5.0397000	-1.8938761
C	0.9948020	3.8226459	-2.5346432
C	0.9269590	2.6209065	-1.8209363
C	0.2278337	3.8473862	0.1774812
C	0.3075455	5.0470284	-0.5391237
H	0.7528175	5.9872565	-2.4544869
H	1.2854998	3.8151227	-3.5979841
H	1.1568459	1.6635327	-2.3166701
H	-0.0799994	3.8505724	1.2334426
H	0.0669994	5.9995647	-0.0392820
C	3.9630695	-4.0219373	1.4494328
C	4.2023586	-3.0250814	0.4899196
C	3.1928921	-2.1067782	0.1579381
C	1.6877952	-3.1905233	1.7206998
C	2.6976743	-4.1047987	2.0573633
H	4.7601895	-4.7329263	1.7225311
H	5.1837171	-2.9583326	-0.0085284
H	3.3961008	-1.3491768	-0.6167166
H	0.7101998	-3.2455799	2.2256543
H	2.4992385	-4.8785330	2.8172817

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-101.84	0.00000	YES	YES
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	19.82	0.04668	YES	YES
9	a	26.78	0.15666	YES	YES
10	a	31.80	0.37669	YES	YES
11	a	40.20	0.20557	YES	YES
12	a	43.70	0.03615	YES	YES
13	a	47.80	0.24022	YES	YES
14	a	53.12	0.20842	YES	YES
15	a	58.20	0.16989	YES	YES
16	a	76.82	0.14507	YES	YES
17	a	88.16	0.32927	YES	YES
18	a	92.55	0.19181	YES	YES
19	a	101.18	0.19223	YES	YES
20	a	115.84	0.51378	YES	YES
21	a	134.32	0.28560	YES	YES
22	a	142.23	0.83050	YES	YES
23	a	169.68	0.93431	YES	YES
24	a	186.56	0.09386	YES	YES
25	a	206.28	1.66894	YES	YES
26	a	229.73	0.47084	YES	YES
27	a	237.12	0.49147	YES	YES
28	a	250.38	1.77895	YES	YES
29	a	261.02	3.38600	YES	YES
30	a	304.35	1.70317	YES	YES
31	a	353.95	5.54405	YES	YES
32	a	390.73	6.44978	YES	YES
33	a	400.70	0.74591	YES	YES
34	a	402.44	0.39983	YES	YES
35	a	403.13	0.39119	YES	YES
36	a	432.59	2.42700	YES	YES
37	a	445.95	6.51090	YES	YES
38	a	453.39	3.00818	YES	YES
39	a	469.58	1.35279	YES	YES
40	a	480.02	0.97809	YES	YES
41	a	484.42	0.28655	YES	YES
42	a	491.23	0.85186	YES	YES
43	a	510.47	5.91320	YES	YES
44	a	521.15	4.56488	YES	YES
45	a	532.73	7.72744	YES	YES
46	a	544.33	11.44481	YES	YES
47	a	556.94	15.98299	YES	YES
48	a	572.11	11.88796	YES	YES
49	a	592.99	11.20011	YES	YES
50	a	610.97	1.19647	YES	YES