Supporting Information for

Time-resolved Infra-red Spectroscopy Reveals Competitive Water and Dinitrogen Coordination to a Manganese(I) Carbonyl Complex

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Contents

1. Determination of Absorption Coefficients for [1].....2

2. Modelling the Ultra-fast Behaviour of [1] on Photolysis in Heptane Solution 4

3. DFT-modelling of heptane binding in [2].....7

4. Behaviour of [1] under Ar. 8

5. Addition of water to heptane 9

6. Collated energies and vibrational spectra. 10

1. Determination of Absorption Coefficients for [1]

A stock solution composed of 18.4 mg of [**1**] was prepared in 100 mL of heptane using volumetric glassware. Using appropriately sized graduated pipettes, this stock was diluted to the following amounts: 25 mL in 50 mL, 12.5 mL in 50 mL, 6.25 mL in 50 mL and 1.1 mL in 100 mL of heptane. The background spectrum of heptane was recorded, using a Specac IR cell with a 100 µm spacer and CaF windows, on a Thermo Nicolet Avatar 370 FTIR instrument (16 scans, resolution of 1 cm^{-1}). Following this background, IR spectra of the of the stock solutions were obtained, with the experiment being repeated in triplicate.

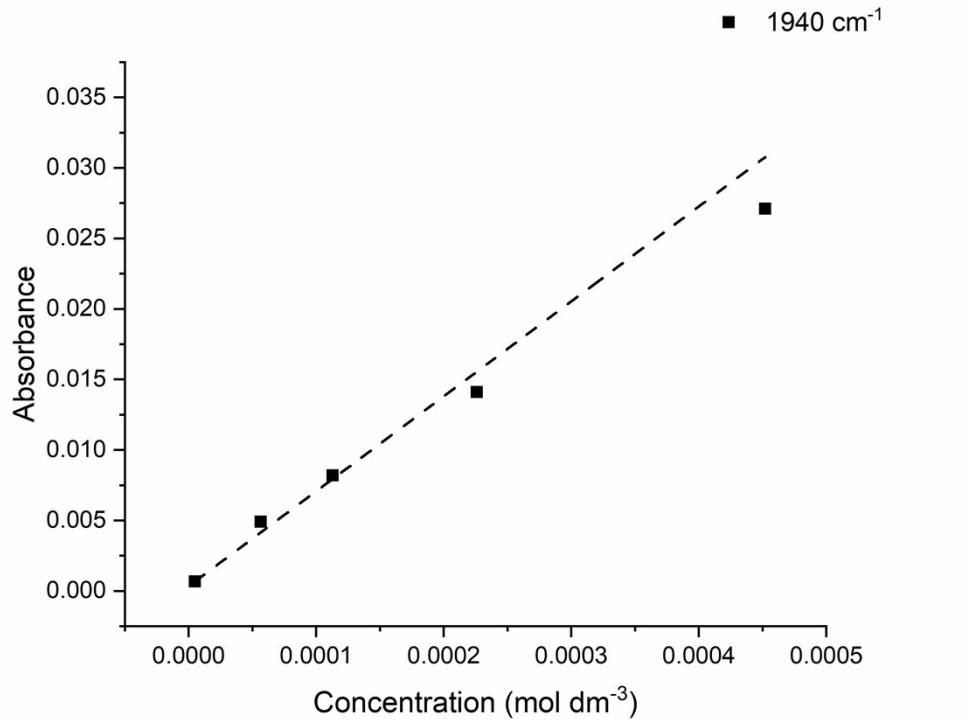

Figure S1. Plot of concentration versus absorbance for a heptane solution of [**1**] monitoring the band at 1940 cm^{-1}. Dashed line shows a fit to the formula $y = 67.3x + 3.38 \times 10^{-4}$ $R^2 = 0.983$.

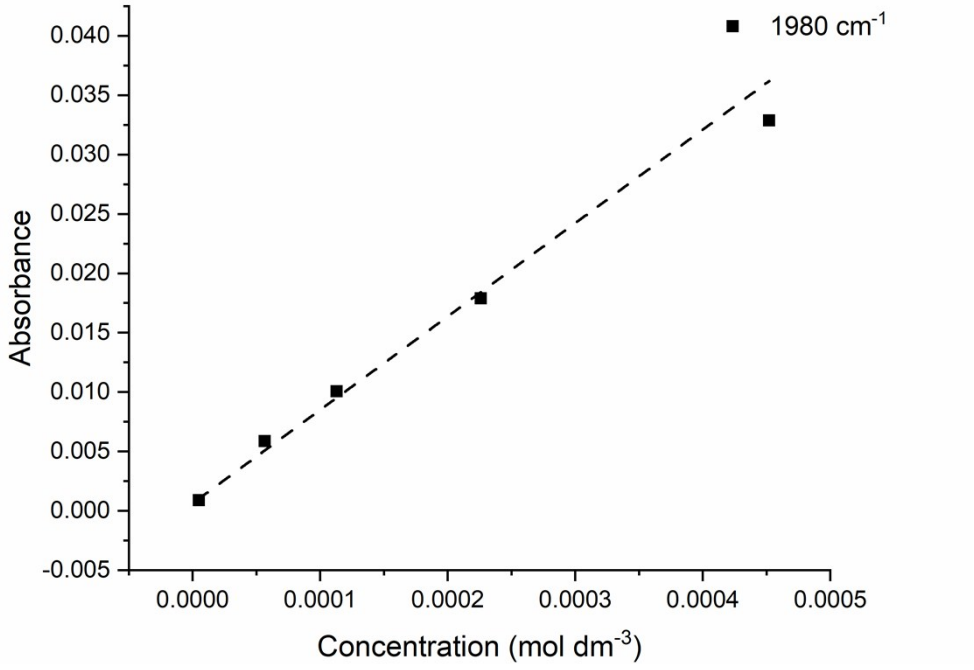

Figure S2. Plot of concentration versus absorbance for a heptane solution of [**1**] monitoring the band at 1980 cm^{-1}. Dashed line shows a fit to the formula $y = 76.6x + 6.32 \times 10^{-4}$ $R^2 = 0.993$

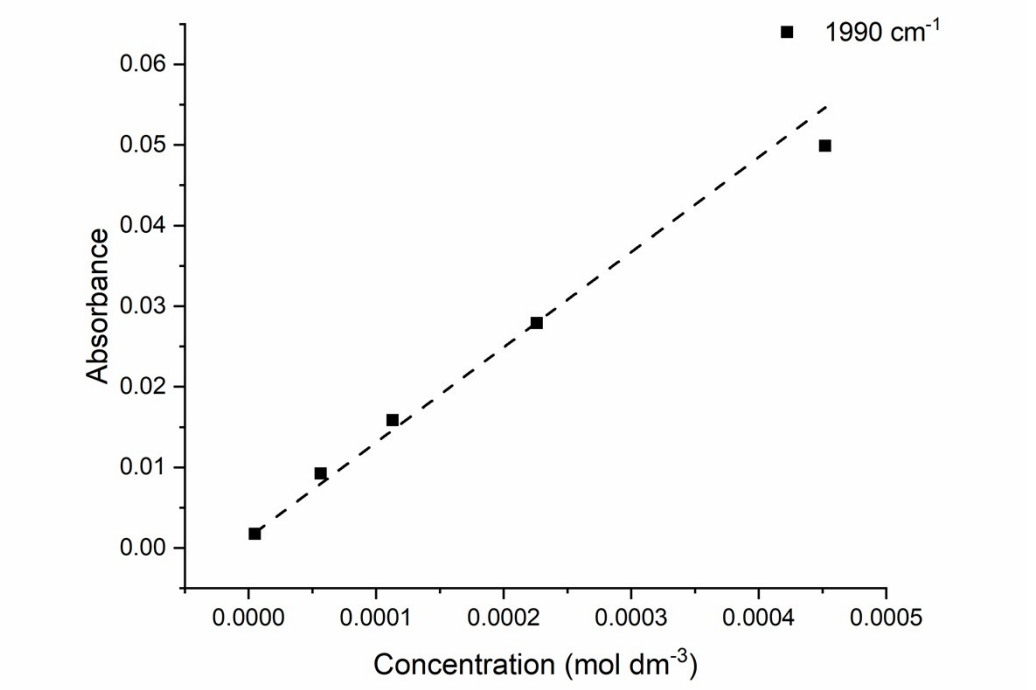

Figure S3. Plot of concentration versus absorbance for a heptane solution of [**1**] monitoring the band at 1990 cm^{-1}. Dashed line shows a fit to the formula $y = 118x + 1.29 \times 10^{-3}$ $R^2 = 0.998$

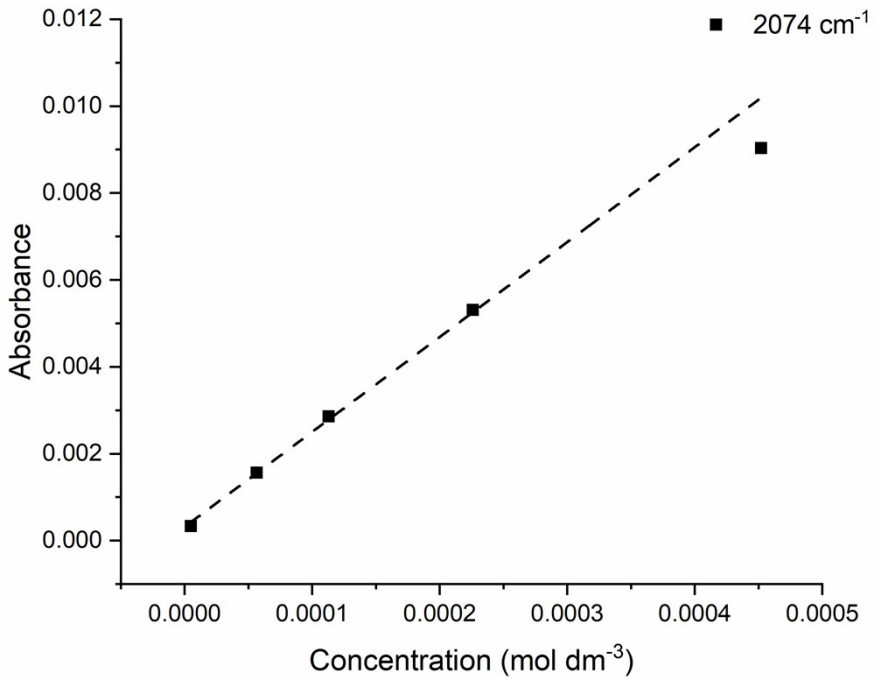

Figure S4. Plot of concentration versus absorbance for a heptane solution of [**1**] monitoring the band at 2074 cm^{-1}. Dashed line shows a fit to the formula $y = 21.84x + 3.17 \times 10^{-4}$ $R^2 = 0.993$

2. Modelling the Ultra-fast Behaviour of [1] on Photolysis in Heptane Solution

Examination of the data acquired following photolysis of [**1**] at short-pump probe delays indicated the formation of the heptane complex, [**2**], ^{3}[**1**] and that the ground state bleach bands recovered in intensity (see Figure 2 in the manuscript).

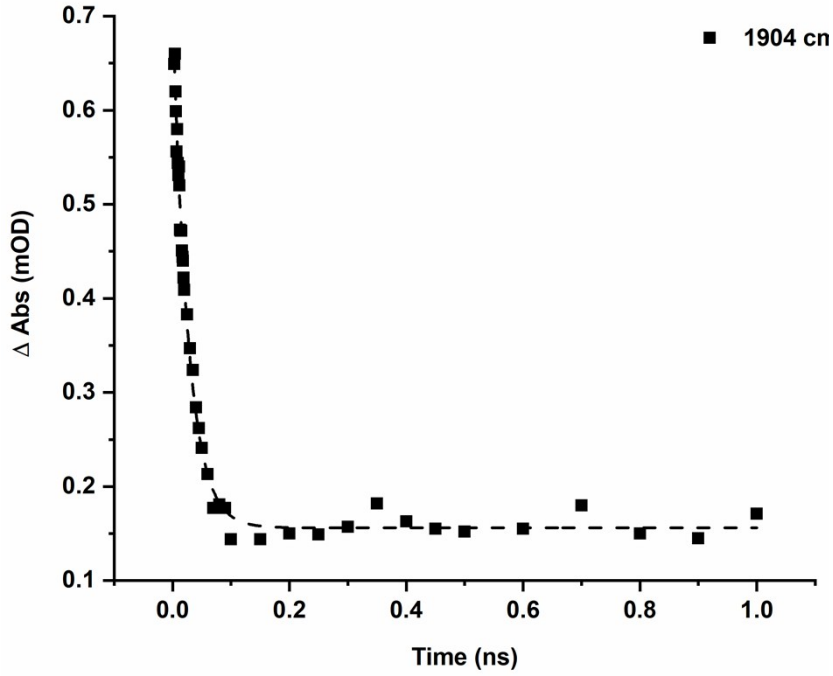

Figure S5. Plot of absorbance versus time for a heptane solution of [**1**] monitoring the band at 1904 cm^{-1} due to the vibrational cooling. Dashed line shows a fit to a monoexponential decay with τ = (26.4 ± 0.8) ps R^2 = 0.995.

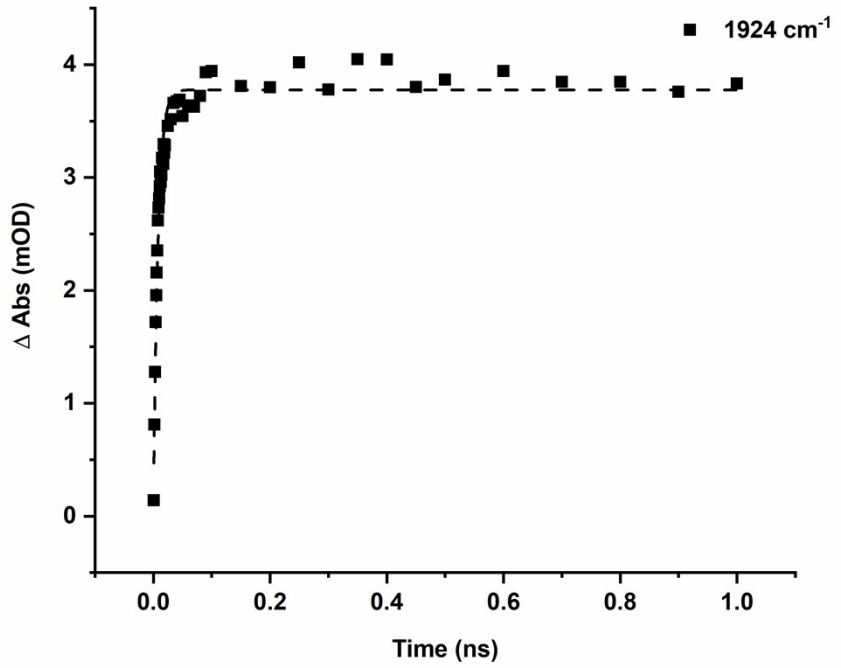

Figure S6. Plot of absorbance versus time for a heptane solution of [**1**] monitoring the band at 1924 cm^{-1}. Dashed line shows a fit to a monoexponential growth with decay with τ = (7.8 ± 0.4) ps R^2 = 0.970.

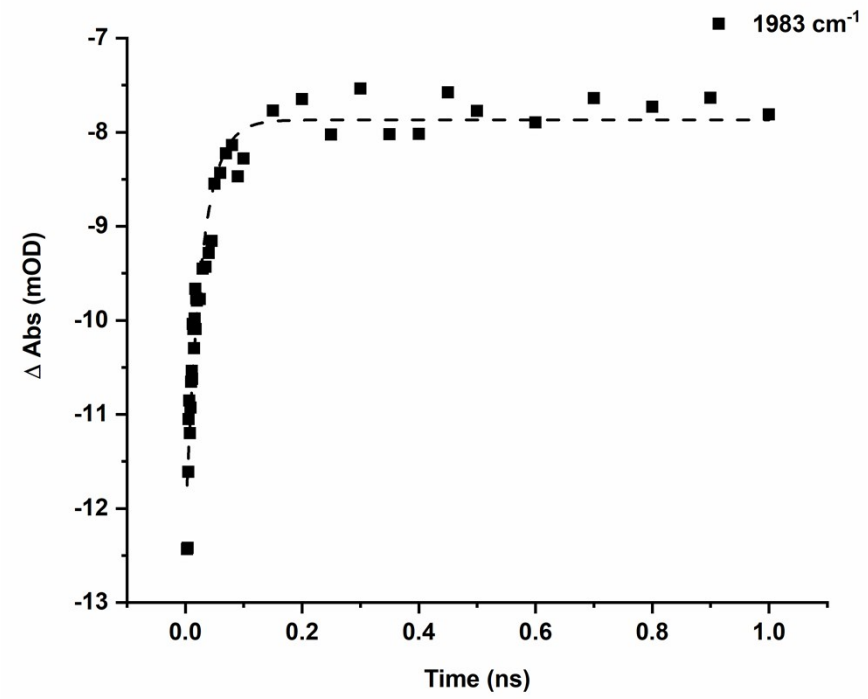

Figure S7. Plot of absorbance versus time for a heptane solution of [**1**] monitoring the band at 1983 cm^{-1} showing recovery of the ground state bleach bands. Dashed line shows a fit to a monoexponential growth with τ = (26.7 ± 2.6) ps R^2 = 0.953.

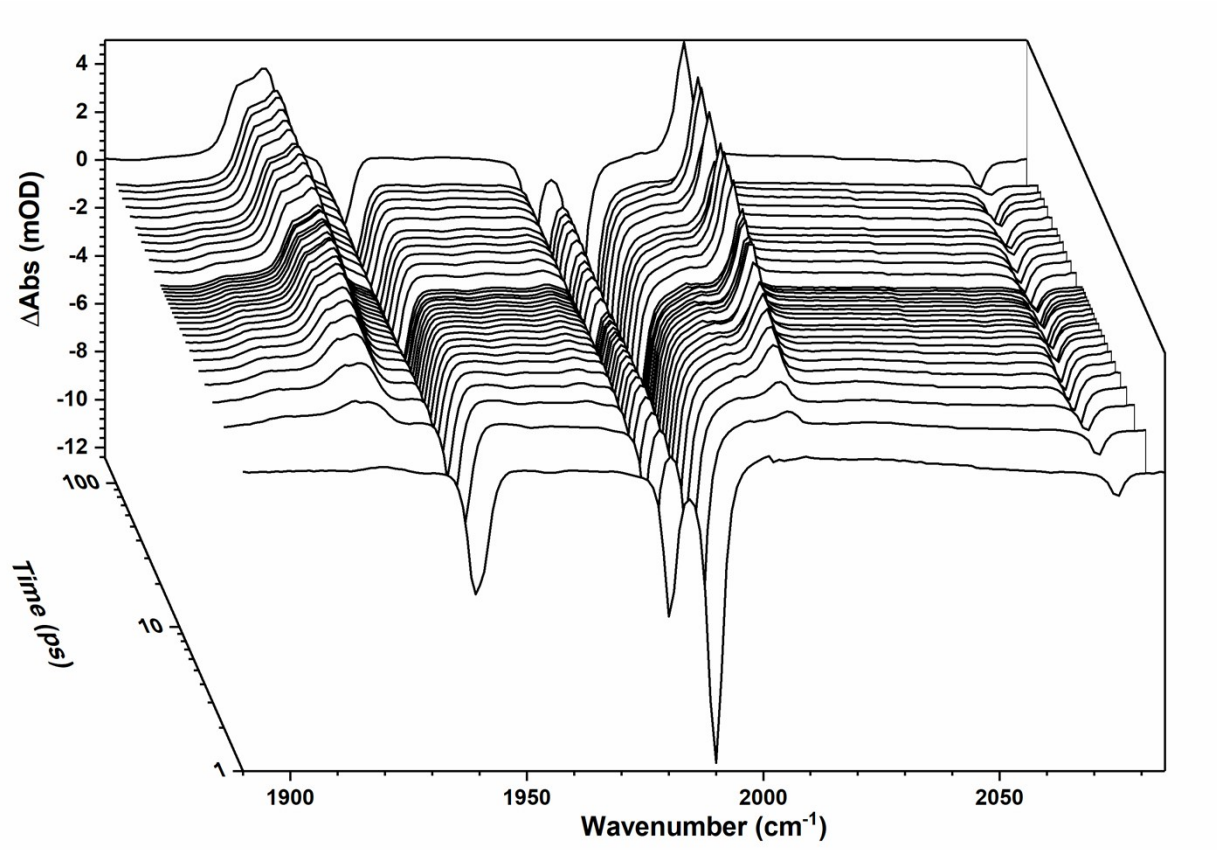

Figure S8. Waterfall plot showing pump-probe delays between 1 and 100 ps. The time axis is a $\log_{10}$ scale.

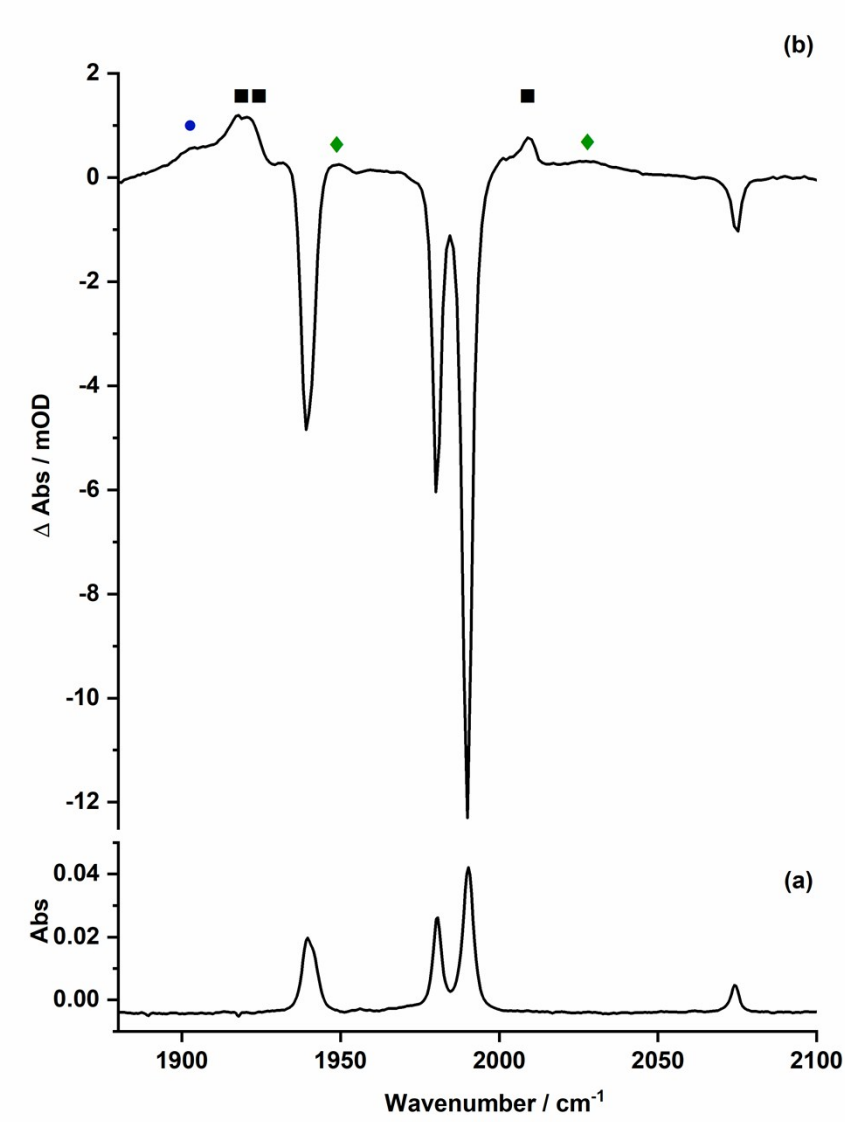

Figure S9. (a) FTIR spectrum of [**1**] in heptane. (b) TRIR spectrum of [**1**] in heptane solution with a pump-probe delay of 2 ps. Black squares show the band positions of [**2**] in the $v = 0$ state, the blue circle for [**2**] in $v > 0$ and green diamonds the bands assigned to ^{3}[**1**].

3. DFT-modelling of heptane binding in [2]

The binding of heptane to [**2**] was modelled at each of the four unique carbon atom sites. The resulting energies, relative to binding to C1, using a range of different DFT-methods are presented in Table S1, the geometries used in all cases were optimised at the BP86/SV(P) level. The greatest difference is for the calculated Gibbs energies for the C2 isomer which correlates with the lower calculated chemical potential for this state, however, given the relatively small value of these differences these data cannot be used to reliably predict which isomer is preferred.

Binding position	Scaled IR modes	BP86/SV(P)		PBE0/def2-TZVPP		PBE0/def2-TZVPP COSMO solvation heptane		D3-PBE0/def2-TZVPP COSMO solvation in heptane	
		$\Delta E_{SCF+ZPE}$	ΔG_{298}	$\Delta E_{SCF+ZPE}$	ΔG_{298}	$\Delta E_{SCF+ZPE}$	ΔG_{298}	$\Delta E_{SCF+ZPE}$	ΔG_{298}
C1	1895 1915 1999	0	0	0	0	0	0	0	0
C2	1896 1914 1998	0	-6	-1	-7	-1	-6	-1	-6
C3	1895 1914 1998	3	2	3	2	3	2	3	2
C4	1895 1914 1998	3	3	3	4	4	4	4	4

Table S1 Calculated energies (kJ mol^{-1}) and scaled IR modes of the carbonyl ligands (cm^{-1}) for the different isomers of heptane complex [**2**].

4. Behaviour of [1] under Ar.

Photolysis of [**1**] under argon results in the initial formation of heptane complex [**2**] (Figure S8b) which, in a similar vein to experiments performed under N_2, transforms to the water complex [**4**] (Figure S8c). At longer times (Figure S8 d) a number of new species are observed that are tentatively assigned to Mn hydroxy-bridged clusters.

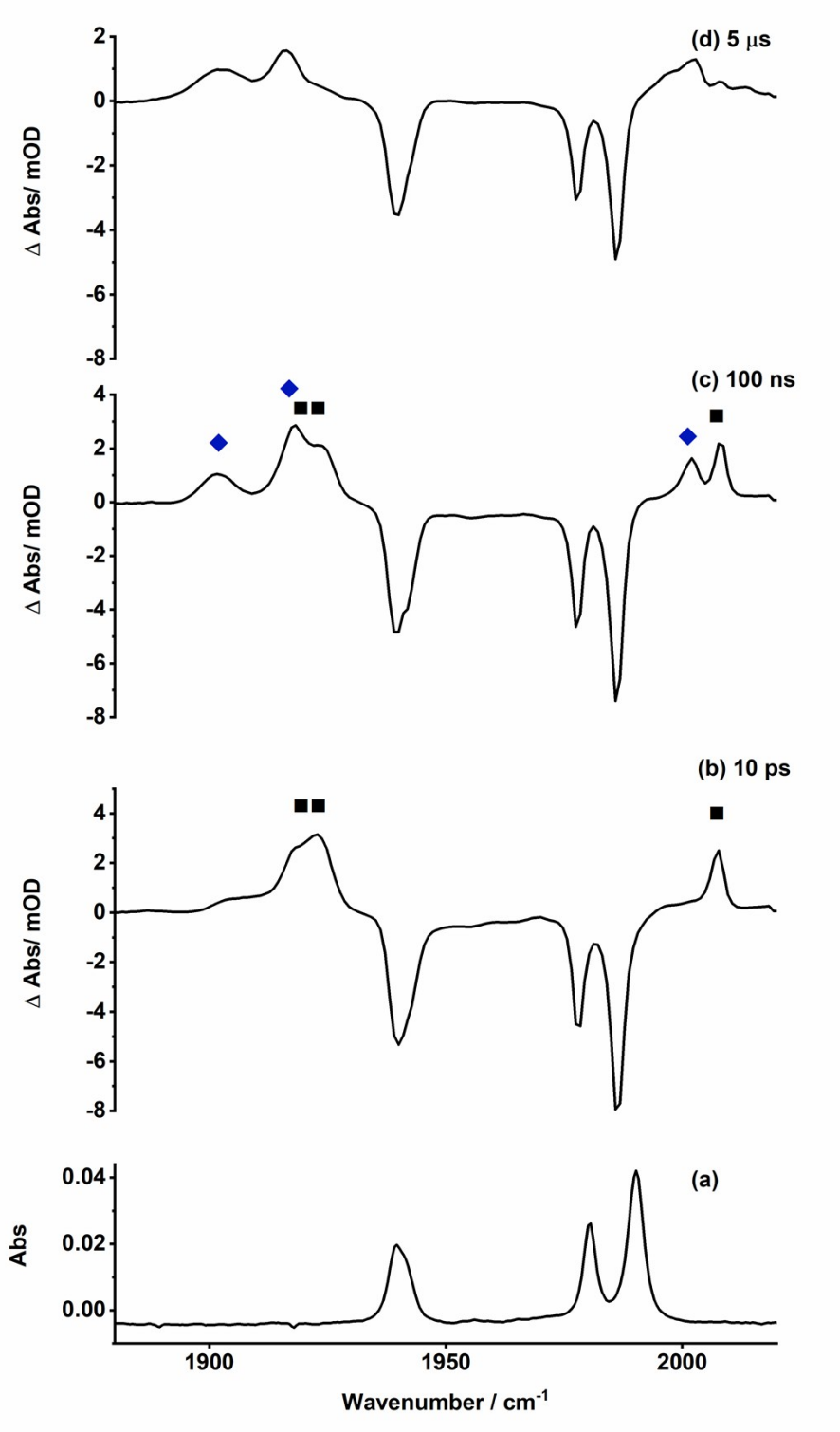

Figure S10. TRIR spectra for the photolysis of [**1**] in heptane solution under Ar (a) ground state spectrum (b) experiment with a pump-probe delay of 10 ps showing the formation of [**2**], black squares. (c) experiment with a pump-probe delay of 100 ns showing the formation of [**2**], black squares and [**4**], blue diamonds. (d) experiment with a pump-probe delay of 5 μs showing the formation of multiple species. Bleach band at 2074 cm^{-1} omitted for clarity.

5. Addition of water to heptane

In order to aid with the assignment of the water complex, [**4**], a sample of [**1**] was photolyzed under an atmosphere of N_2 (Figure S9b). A single drop of water was then added to the sample and the experiment repeated (Figure S9c) demonstrating an increase in the amount of [**4**] (blue diamonds) relative to [**3**] (red circles).

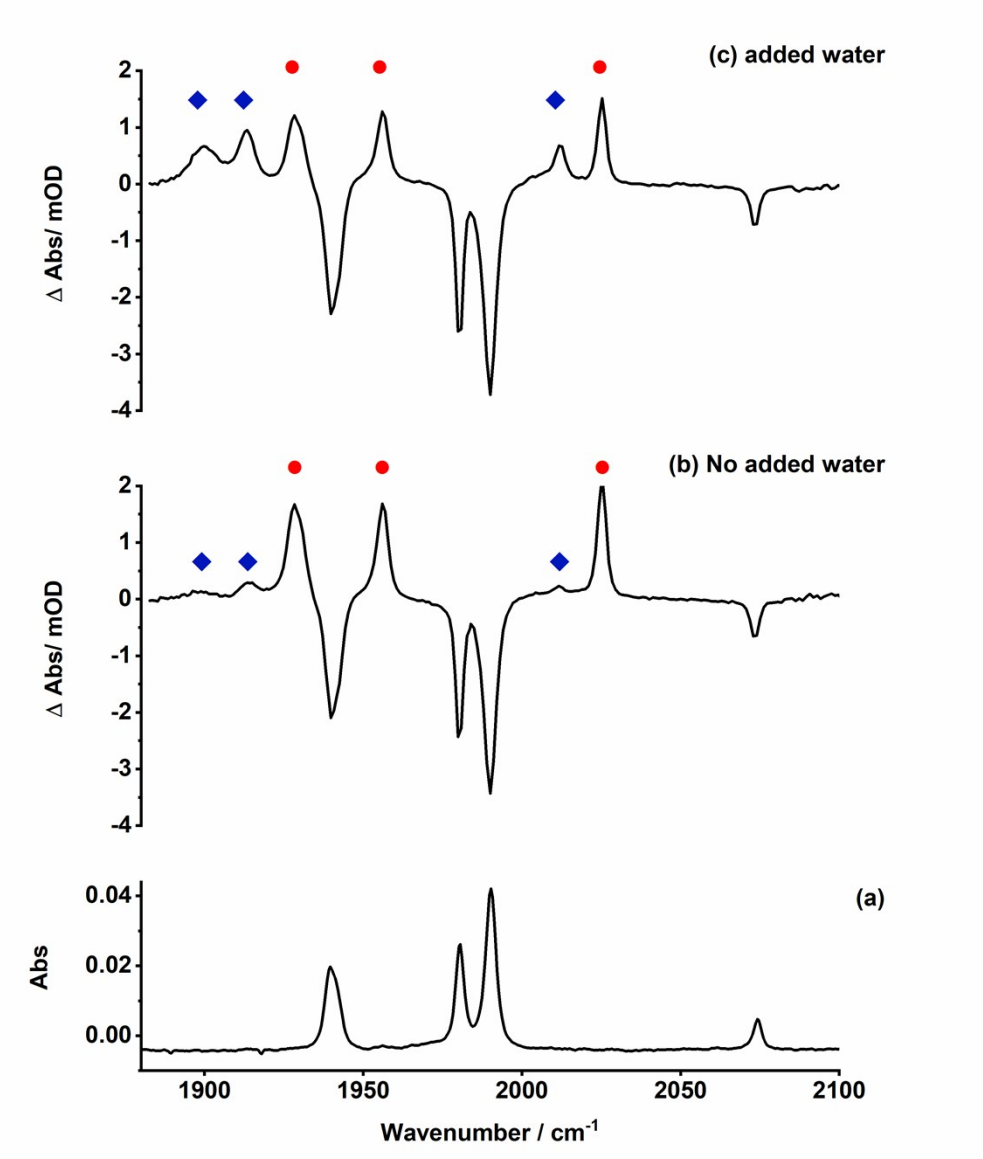

Figure S11. TRIR spectra for the photolysis of [**1**] in heptane solution under N_2 (a) ground state spectrum (b) experiment with a pump-probe delay of 1 μs showing that dinitrogen complex [**3**], red circles, is the dominant product. (c) experiment repeated with a single drop of water added to the sample showing an increase in the proportion of [**4**], blue diamonds.

6. Collated energies and vibrational spectra.

[**1**]

SCF Energy (au) BP86/SV(P)	-2388.8496391370
SCF Energy (au) PBE0/def2-TZVPP	-2388.444541898
Zero Point Energy (au)	0.2863571
Chemical potential (kJ mol^{-1})	599.73
Dispersion correction (au) PBE0/def2-TZVPP	-0.05312021
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-2388.4508474159

xyz coordinates

41

Mn	3.32923	0.73855	0.37598
C	3.03571	0.34890	2.15038
C	4.04822	2.38844	0.66001
O	4.49964	3.44838	0.83629
O	2.83984	0.07117	3.25919
C	0.42767	0.67014	0.02240
C	-0.95715	1.19041	-0.09500
C	0.80767	-0.74215	-0.08668
C	2.21473	-0.98045	0.02998
C	2.63630	-2.31749	-0.06017
C	1.72699	-3.37974	-0.24620
C	0.34054	-3.12450	-0.33331
C	-0.11667	-1.79584	-0.24630
N	1.43665	1.47958	0.25298
C	4.90674	-0.12703	0.45045
O	5.91695	-0.70746	0.49806
C	3.45337	0.79463	-1.45964
H	-1.20183	-1.61594	-0.28885
O	-0.62155	-4.08229	-0.49287
H	2.11588	-4.40759	-0.31026
H	3.70732	-2.56945	0.01972
C	-3.57290	2.27998	-0.32946
C	-3.08603	1.36337	-1.29213
C	-1.80495	0.82338	-1.17197
C	-1.45075	2.11405	0.85280
C	-2.74224	2.65324	0.75081
O	-4.83540	2.73854	-0.52868
H	-3.74160	1.09413	-2.13497
H	-1.43862	0.12836	-1.94396
H	-0.82203	2.39730	1.71380
H	-3.09253	3.35360	1.52301
H	1.19084	2.47875	0.29570
O	3.52707	0.79006	-2.61692
C	-0.22058	-5.43771	-0.57187
C	-5.38847	3.65857	0.40036
H	-5.45681	3.21903	1.42323
H	-6.40951	3.88654	0.03438
H	-4.79749	4.60344	0.44550
H	0.30203	-5.77206	0.35638
H	0.44505	-5.62472	-1.44855
H	-1.15134	-6.02811	-0.69358

$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	26.28	0.06802	YES	YES
8	a	34.69	0.47769	YES	YES
9	a	40.02	0.12265	YES	YES
10	a	52.68	0.78137	YES	YES
11	a	58.24	1.14003	YES	YES
12	a	72.22	0.63734	YES	YES
13	a	75.24	0.01637	YES	YES
14	a	81.70	0.93070	YES	YES
15	a	88.72	0.24597	YES	YES
16	a	90.82	0.02692	YES	YES
17	a	92.32	0.24563	YES	YES
18	a	99.17	0.38075	YES	YES
19	a	103.61	1.97811	YES	YES
20	a	129.04	1.51717	YES	YES
21	a	151.98	1.82135	YES	YES
22	a	178.24	1.50336	YES	YES
23	a	193.64	0.83460	YES	YES
24	a	211.05	1.02871	YES	YES
25	a	225.74	1.16918	YES	YES
26	a	245.91	0.22522	YES	YES
27	a	247.02	0.10912	YES	YES
28	a	250.95	0.67806	YES	YES
29	a	294.27	1.80392	YES	YES
30	a	319.99	3.92586	YES	YES
31	a	324.46	2.16673	YES	YES
32	a	354.63	1.79935	YES	YES
33	a	414.96	1.81219	YES	YES
34	a	418.86	0.77315	YES	YES
35	a	431.55	2.06704	YES	YES
36	a	434.43	1.15552	YES	YES
37	a	437.14	0.80613	YES	YES
38	a	446.39	0.12778	YES	YES
39	a	459.37	1.70816	YES	YES
40	a	476.35	0.37541	YES	YES
41	a	490.23	2.63363	YES	YES
42	a	493.04	15.29233	YES	YES
43	a	500.78	1.89126	YES	YES
44	a	512.47	13.55587	YES	YES
45	a	512.68	4.93768	YES	YES
46	a	544.58	9.01692	YES	YES
47	a	548.18	19.14965	YES	YES
48	a	569.25	2.10998	YES	YES
49	a	572.39	6.23530	YES	YES
50	a	579.52	19.55305	YES	YES

[**2**] C1-bound

SCF Energy (au) BP86/SV(P)	-2551.7199143720
SCF Energy (au) PBE0/def2-TZVPP	-2551.303778446
Zero Point Energy (au)	0.4894833
Chemical potential (kJ mol^{-1})	1093.94
Dispersion correction (au) PBE0/def2-TZVPP	-0.07346752
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-2551.3108730575

xyz coordinates

62

Mn	1.23664	0.78240	1.65236
C	1.63942	0.50321	3.34122
C	1.67891	2.55128	1.69516
O	1.98397	3.67835	1.74814
O	1.88610	0.29541	4.46412
C	-1.57233	0.12465	1.96359
C	-3.02530	0.35067	2.15157
C	-0.94229	-1.18475	1.74434
C	0.47928	-1.11963	1.56123
C	1.13086	-2.35434	1.38600
C	0.44127	-3.58696	1.38168
C	-0.95489	-3.61866	1.57986
C	-1.64660	-2.40438	1.76893
N	-0.71789	1.12558	2.00249
C	2.88081	0.24949	1.17388
O	3.95077	-0.11971	0.87776
H	1.02701	0.59841	-0.32523
H	-2.73053	-2.45143	1.95470
O	-1.71707	-4.75318	1.61541
H	1.01145	-4.51779	1.23854
H	2.22574	-2.38747	1.25059
C	-5.79775	0.88687	2.49408
C	-5.35159	0.04364	1.44821
C	-3.99199	-0.22470	1.28606
C	-3.48380	1.19961	3.18434
C	-4.84904	1.46553	3.36699
O	-7.13986	1.07564	2.57529
H	-6.10321	-0.38824	0.76915
H	-3.66576	-0.86560	0.45195
H	-2.75778	1.63911	3.88895
H	-5.16170	2.11548	4.19715
H	-1.14870	2.05035	2.14583
C	0.44206	1.22127	-1.07121
C	-1.07272	-6.00462	1.46404
C	-7.65674	1.91454	3.59762
H	-7.41455	1.52218	4.61322
H	-8.75679	1.91856	3.46302
H	-7.27364	2.95797	3.50628
H	-0.32061	-6.18493	2.26899
H	-0.56821	-6.09594	0.47215
H	-1.86953	-6.77277	1.53540
H	-0.20177	0.46942	-1.58136
C	1.40474	1.91929	-2.03542
H	-0.22088	1.93882	-0.54756
C	2.38194	0.96209	-2.73650
H	1.97980	2.69774	-1.48298
H	0.80573	2.46832	-2.80055
H	2.97880	0.42100	-1.96446

C	3.33670	1.66235	-3.71555
H	1.80316	0.17789	-3.28113
C	4.33071	0.71027	-4.39946
H	3.90317	2.45466	-3.17034
H	2.74062	2.19639	-4.49437
H	4.92746	0.18018	-3.61892
C	5.28663	1.40783	-5.38043
H	3.76568	-0.08599	-4.94145
C	6.28261	0.45219	-6.05062
H	5.84562	2.20735	-4.83924
H	4.68955	1.93293	-6.16329
H	6.92446	-0.05782	-5.29680
H	6.95517	0.99102	-6.75434
H	5.75668	-0.34105	-6.62904

$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	7.27	0.03682	YES	YES
8	a	11.82	0.24791	YES	YES
9	a	25.51	0.32182	YES	YES
10	a	31.38	0.20117	YES	YES
11	a	35.63	0.72967	YES	YES
12	a	43.22	0.01522	YES	YES
13	a	53.86	0.71777	YES	YES
14	a	56.58	1.24905	YES	YES
15	a	62.22	0.29767	YES	YES
16	a	65.92	0.05641	YES	YES
17	a	72.90	0.20854	YES	YES
18	a	77.47	0.26418	YES	YES
19	a	83.75	0.80139	YES	YES
20	a	88.81	1.11943	YES	YES
21	a	90.57	0.43031	YES	YES
22	a	94.05	0.09487	YES	YES
23	a	100.09	1.99731	YES	YES
24	a	102.34	1.57240	YES	YES
25	a	118.67	0.45505	YES	YES
26	a	131.19	1.12809	YES	YES
27	a	136.03	0.25764	YES	YES
28	a	150.98	1.03148	YES	YES
29	a	155.46	0.81716	YES	YES
30	a	177.63	0.37264	YES	YES
31	a	190.86	2.26955	YES	YES
32	a	199.68	3.77640	YES	YES
33	a	213.78	2.23016	YES	YES
34	a	227.25	1.24998	YES	YES
35	a	241.96	0.15861	YES	YES
36	a	244.26	0.22319	YES	YES
37	a	246.30	0.09537	YES	YES
38	a	251.32	0.16376	YES	YES
39	a	253.61	1.53694	YES	YES
40	a	292.21	1.53549	YES	YES

41	a	302.41	0.15238	YES	YES
42	a	318.31	4.37346	YES	YES
43	a	323.04	1.74756	YES	YES
44	a	355.43	2.25980	YES	YES
45	a	377.72	7.92593	YES	YES
46	a	415.87	3.51190	YES	YES
47	a	424.74	0.35263	YES	YES
48	a	427.19	9.07822	YES	YES
49	a	436.83	0.62277	YES	YES
50	a	453.07	1.21352	YES	YES

[**2**] C2-bound

SCF Energy (au) BP86/SV(P)	-2551.7194387730
SCF Energy (au) PBE0/def2-TZVPP	-2551.303681931
Zero Point Energy (au)	0.4888863
Chemical potential (kJ mol^{-1})	1086.78
Dispersion correction (au) PBE0/def2-TZVPP	-0.07658720
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-2551.3105670166

xyz coordinates

62

Mn	1.97078	1.44794	1.40235
C	2.52608	0.95084	2.99376
C	2.28369	3.21534	1.71492
O	2.50112	4.33868	1.95505
O	2.87565	0.59787	4.05162
C	-0.75699	0.52106	1.76108
C	-2.21049	0.60559	2.03708
C	-0.04348	-0.69332	1.34238
C	1.35299	-0.48296	1.08705
C	2.08678	-1.62980	0.72930
C	1.49832	-2.90866	0.61444
C	0.12477	-3.08355	0.88340
C	-0.64654	-1.96358	1.25739
N	0.02174	1.57592	1.89143
C	3.59576	1.13757	0.70987
O	4.65075	0.91275	0.25876
H	2.11809	2.88004	-1.30174
H	-1.70862	-2.12554	1.49810
O	-0.54113	-4.27582	0.82317
H	2.13101	-3.76355	0.32943
H	3.17026	-1.55263	0.53246
C	-4.99404	0.88993	2.54843
C	-4.54060	0.20603	1.39480
C	-3.17491	0.06051	1.14930
C	-2.67742	1.29257	3.18093
C	-4.04747	1.43255	3.44668
O	-6.34040	0.97035	2.70219
H	-5.29173	-0.20010	0.69959
H	-2.84451	-0.45445	0.23351
H	-1.95122	1.70090	3.90376
H	-4.36521	1.95653	4.35987
H	-0.47127	2.43843	2.16424
C	1.14541	2.34250	-1.32053
C	0.18764	-5.44021	0.48055
C	-6.86498	1.65139	3.83249
H	-6.55233	1.16592	4.78671
H	-7.96784	1.59332	3.73997
H	-6.55522	2.72271	3.84714
H	1.00329	-5.65027	1.21311
H	0.63039	-5.36817	-0.54178
H	-0.54008	-6.27681	0.50059
H	1.13405	1.62423	-0.43950
C	1.06331	1.47319	-2.58606
C	-0.00924	3.33818	-1.17616
C	2.22522	0.48310	-2.75411
H	1.02516	2.15624	-3.46954
H	0.09570	0.91743	-2.58793
H	3.19203	1.03932	-2.72725

C	2.14772	-0.34233	-4.04814
H	2.24432	-0.20551	-1.87738
C	3.30486	-1.34112	-4.21474
H	2.12739	0.34629	-4.92775
H	1.17840	-0.89632	-4.07401
H	4.27283	-0.78730	-4.18901
H	3.32502	-2.02510	-3.33368
H	0.10993	3.97613	-0.27449
H	-0.99090	2.81864	-1.10645
C	3.22207	-2.16805	-5.50450
H	-0.05125	4.01314	-2.06086
H	4.07581	-2.87633	-5.59166
H	3.23592	-1.51502	-6.40678
H	2.28360	-2.76665	-5.54286

$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		0.73	0.10916	-	-
8	a	16.64	0.05337	YES	YES
9	a	24.11	0.29143	YES	YES
10	a	32.56	0.24720	YES	YES
11	a	35.62	0.68846	YES	YES
12	a	46.51	0.15164	YES	YES
13	a	51.31	0.08562	YES	YES
14	a	55.55	1.86219	YES	YES
15	a	58.69	0.05401	YES	YES
16	a	71.37	0.01969	YES	YES
17	a	72.62	0.02861	YES	YES
18	a	75.66	0.61464	YES	YES
19	a	80.60	0.61783	YES	YES
20	a	84.86	1.10990	YES	YES
21	a	89.35	1.38122	YES	YES
22	a	92.45	0.11420	YES	YES
23	a	98.30	1.54393	YES	YES
24	a	102.41	1.46386	YES	YES
25	a	111.29	0.11156	YES	YES
26	a	126.35	1.11360	YES	YES
27	a	134.33	0.04066	YES	YES
28	a	145.71	0.05873	YES	YES
29	a	151.80	1.77333	YES	YES
30	a	169.95	0.11282	YES	YES
31	a	180.64	2.71230	YES	YES
32	a	191.91	0.47184	YES	YES
33	a	212.00	0.58769	YES	YES
34	a	224.34	0.99550	YES	YES
35	a	240.36	0.33760	YES	YES
36	a	243.45	0.31600	YES	YES
37	a	246.44	3.11874	YES	YES
38	a	249.58	0.03506	YES	YES
39	a	252.87	0.75665	YES	YES
40	a	262.82	1.35694	YES	YES
41	a	292.95	1.91221	YES	YES

42	a	299.56	0.07319	YES	YES
43	a	316.96	7.17521	YES	YES
44	a	322.06	1.72922	YES	YES
45	a	354.94	2.27234	YES	YES
46	a	412.74	1.29859	YES	YES
47	a	415.86	3.66564	YES	YES
48	a	425.80	2.86135	YES	YES
49	a	436.42	0.71545	YES	YES
50	a	447.66	0.60889	YES	YES

[**2**] C3-bound

SCF Energy (au) BP86/SV(P)	-2551.7181555600
SCF Energy (au) PBE0/def2-TZVPP	-2551.302200705
Zero Point Energy (au)	0.4889881
Chemical potential (kJ mol^{-1})	1091.63
Dispersion correction (au) PBE0/def2-TZVPP	-0.07732848
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-2551.3090842390

xyz coordinates

62

Mn	2.12909	1.09565	1.22133
C	2.69715	0.59569	2.80682
C	2.44551	2.86224	1.53701
O	2.66877	3.98361	1.78092
O	3.05566	0.24014	3.86085
C	-0.59570	0.16505	1.59259
C	-2.04849	0.24764	1.87243
C	0.11780	-1.04822	1.17093
C	1.51284	-0.83581	0.90981
C	2.24746	-1.98232	0.55255
C	1.66103	-3.26253	0.44287
C	0.28864	-3.43917	0.71660
C	-0.48340	-2.31965	1.09050
N	0.18255	1.22052	1.72183
C	3.74930	0.78895	0.51659
O	4.80206	0.56695	0.05875
H	2.26284	2.55862	-1.47142
H	-1.54433	-2.48295	1.33537
O	-0.37528	-4.63277	0.66162
H	2.29433	-4.11698	0.15794
H	3.33007	-1.90357	0.35160
C	-4.83136	0.52761	2.38977
C	-4.37937	-0.15561	1.23518
C	-3.01399	-0.29898	0.98675
C	-2.51399	0.93397	3.01725
C	-3.88369	1.07175	3.28597
O	-6.17753	0.60600	2.54639
H	-5.13137	-0.56279	0.54153
H	-2.68465	-0.81324	0.07020
H	-1.78691	1.34338	3.73857
H	-4.20029	1.59519	4.19987
H	-0.31049	2.08223	1.99709
C	1.28997	2.01985	-1.50725
C	0.35479	-5.79688	0.32068
C	-6.70077	1.28612	3.67785
H	-6.38531	0.80108	4.63136
H	-7.80373	1.22634	3.58764
H	-6.39270	2.35794	3.69194
H	1.17285	-6.00296	1.05169
H	0.79460	-5.72724	-0.70307
H	-0.37126	-6.63479	0.34539
H	1.26522	1.29916	-0.62878
C	1.22784	1.15199	-2.77515
C	0.13479	3.02364	-1.33991
C	2.36869	0.13096	-2.89843
H	1.24373	1.82270	-3.66677
H	0.24673	0.62071	-2.80671
H	3.34852	0.66122	-2.83685

C	2.31754	-0.69472	-4.19408
H	2.33821	-0.55645	-2.02103
C	3.45013	-1.72398	-4.30592
H	2.35205	-0.00654	-5.07233
H	1.33349	-1.21716	-4.25644
H	4.44856	-1.23166	-4.28320
H	3.41926	-2.44946	-3.46179
C	0.08177	4.11364	-2.42123
H	0.23423	3.51188	-0.34444
H	-0.83332	2.47001	-1.31948
H	3.38248	-2.30482	-5.25250
H	1.04030	4.67820	-2.47090
H	-0.72695	4.84571	-2.20392
H	-0.11598	3.69493	-3.43241

$vibrational spectrum

#		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	6.35	0.07389	YES	YES
8	a	18.79	0.11719	YES	YES
9	a	18.99	0.17564	YES	YES
10	a	34.26	0.33753	YES	YES
11	a	35.93	0.41086	YES	YES
12	a	43.00	0.08521	YES	YES
13	a	48.89	0.31692	YES	YES
14	a	55.53	1.93094	YES	YES
15	a	60.24	0.04943	YES	YES
16	a	63.00	0.10075	YES	YES
17	a	72.38	0.02480	YES	YES
18	a	76.34	0.55950	YES	YES
19	a	82.05	1.07192	YES	YES
20	a	83.53	0.02464	YES	YES
21	a	85.82	1.42316	YES	YES
22	a	89.39	1.12568	YES	YES
23	a	92.65	0.08661	YES	YES
24	a	98.52	1.37699	YES	YES
25	a	102.83	1.58841	YES	YES
26	a	126.91	0.17471	YES	YES
27	a	130.44	0.72271	YES	YES
28	a	145.18	0.18262	YES	YES
29	a	151.70	1.81574	YES	YES
30	a	173.99	0.10323	YES	YES
31	a	181.96	3.29031	YES	YES
32	a	191.71	0.47772	YES	YES
33	a	212.16	0.65412	YES	YES
34	a	224.33	0.92663	YES	YES
35	a	233.25	0.35715	YES	YES
36	a	241.09	0.38898	YES	YES
37	a	243.57	0.31254	YES	YES
38	a	249.31	0.01357	YES	YES
39	a	250.76	2.67853	YES	YES
40	a	291.76	1.55553	YES	YES
41	a	300.52	1.10581	YES	YES
42	a	316.34	6.58359	YES	YES

43	a	321.98	1.64023	YES	YES
44	a	352.15	1.28242	YES	YES
45	a	355.40	2.53186	YES	YES
46	a	393.27	2.54438	YES	YES
47	a	415.82	3.79555	YES	YES
48	a	425.89	3.02858	YES	YES
49	a	436.39	0.77977	YES	YES
50	a	447.36	0.62194	YES	YES

[**2**] C4-bound

SCF Energy (au) BP86/SV(P)	-2551.7183217140
SCF Energy (au) PBE0/def2-TZVPP	-2551.301959507
Zero Point Energy (au)	0.4889275
Chemical potential (kJ mol^{-1})	1092.74
Dispersion correction (au) PBE0/def2-TZVPP	-0.07693777
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-2551.3088316523

xyz coordinates

62

Mn	2.20762	0.61221	1.56585
C	2.48624	0.07381	3.21469
C	2.50588	2.36568	1.97514
O	2.71856	3.47627	2.26950
O	2.64937	-0.30741	4.30747
C	-0.55362	-0.25549	1.40782
C	-2.03122	-0.15554	1.45880
C	0.19985	-1.45724	1.02299
C	1.62333	-1.27425	1.03234
C	2.38547	-2.41310	0.71164
C	1.80186	-3.65954	0.39246
C	0.39978	-3.80960	0.40702
C	-0.40340	-2.69677	0.73350
N	0.20963	0.76534	1.74077
C	3.91696	0.25898	1.16512
O	5.02903	-0.00850	0.91894
H	2.17446	1.36258	-0.37583
H	-1.49383	-2.84220	0.77374
O	-0.26861	-4.97079	0.13643
H	2.45781	-4.51006	0.15078
H	3.48779	-2.35805	0.70980
C	-4.85891	0.13809	1.56330
C	-4.23808	-0.45680	0.43867
C	-2.85184	-0.60772	0.39234
C	-2.66351	0.44720	2.57015
C	-4.05735	0.59035	2.63572
O	-6.21275	0.22686	1.51850
H	-4.87632	-0.79090	-0.39418
H	-2.38907	-1.05297	-0.50252
H	-2.05404	0.78259	3.42605
H	-4.50747	1.04496	3.53013
H	-0.30641	1.61694	2.00521
C	1.52087	1.45436	-1.30171
C	0.48598	-6.12882	-0.17004
C	-6.90070	0.81816	2.61097
H	-6.73486	0.25081	3.55695
H	-7.97729	0.78156	2.35057
H	-6.59711	1.88098	2.76135
H	1.15838	-6.42124	0.67176
H	1.10085	-5.99275	-1.09213
H	-0.24995	-6.94001	-0.34355
H	0.82315	0.58673	-1.28158
C	2.45183	1.34680	-2.51997
C	0.73530	2.77285	-1.19922
C	3.28930	0.06005	-2.57830
H	3.13003	2.23383	-2.54214
H	1.83302	1.41453	-3.44624
H	3.93971	0.00301	-1.67636

C	4.15762	-0.03782	-3.83964
H	2.61117	-0.82307	-2.51907
H	4.87036	0.81531	-3.90916
H	3.53622	-0.02831	-4.76418
C	-0.27692	3.01269	-2.33428
H	1.45187	3.62741	-1.15500
H	0.18792	2.78443	-0.22893
H	0.25458	3.07225	-3.31151
C	-1.10812	4.28787	-2.13652
H	-0.95784	2.13162	-2.40898
H	-1.82678	4.43932	-2.97212
H	-0.45800	5.19059	-2.08499
H	-1.69483	4.24672	-1.19091
H	4.75703	-0.97477	-3.84739

$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	14.07	0.01889	YES	YES
8	a	16.13	0.13217	YES	YES
9	a	19.35	0.03958	YES	YES
10	a	34.67	0.63202	YES	YES
11	a	36.63	0.15900	YES	YES
12	a	42.53	0.43165	YES	YES
13	a	54.74	0.27667	YES	YES
14	a	56.29	1.64411	YES	YES
15	a	59.03	0.09053	YES	YES
16	a	60.52	0.17536	YES	YES
17	a	67.16	0.14862	YES	YES
18	a	73.23	0.18122	YES	YES
19	a	77.93	0.08385	YES	YES
20	a	80.89	0.54395	YES	YES
21	a	85.81	0.64288	YES	YES
22	a	90.40	1.43434	YES	YES
23	a	94.30	0.12786	YES	YES
24	a	97.82	0.73914	YES	YES
25	a	100.69	1.74535	YES	YES
26	a	105.00	2.29501	YES	YES
27	a	130.87	0.66367	YES	YES
28	a	146.75	0.15773	YES	YES
29	a	152.43	1.81896	YES	YES
30	a	179.34	1.69518	YES	YES
31	a	191.78	0.74314	YES	YES
32	a	210.44	0.86256	YES	YES
33	a	213.00	1.26049	YES	YES
34	a	226.28	0.91061	YES	YES
35	a	235.29	0.15628	YES	YES
36	a	245.56	0.45273	YES	YES
37	a	247.07	0.37149	YES	YES
38	a	248.71	0.10859	YES	YES
39	a	252.08	2.90686	YES	YES
40	a	286.18	2.17921	YES	YES
41	a	293.12	1.47647	YES	YES

42	a	302.74	0.40262	YES	YES
43	a	315.06	3.01567	YES	YES
44	a	322.38	1.94383	YES	YES
45	a	356.18	2.19840	YES	YES
46	a	398.35	1.63128	YES	YES
47	a	415.44	3.69951	YES	YES
48	a	424.85	2.09348	YES	YES
49	a	437.15	1.00122	YES	YES
50	a	449.04	0.44123	YES	YES

[**3**]

SCF Energy (au) BP86/SV(P)	-2385.0365037980
SCF Energy (au) PBE0/def2-TZVPP	-2384.626651427
Zero Point Energy (au)	0.2863196
Chemical potential (kJ mol^{-1})	600.05
Dispersion correction (au) PBE0/def2-TZVPP	-0.05305957
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-2384.6329131839

xyz coordinates
41

Mn	3.32844	0.73210	0.36884
C	3.09055	0.35002	2.11979
C	4.07613	2.36967	0.69088
O	4.54815	3.40905	0.92717
O	2.92007	0.08567	3.23858
C	0.43161	0.66481	0.03032
C	-0.95291	1.18408	-0.09420
C	0.81200	-0.74915	-0.07438
C	2.21696	-0.99022	0.06236
C	2.63132	-2.33032	-0.00851
C	1.72115	-3.39066	-0.20735
C	0.33845	-3.12997	-0.32185
C	-0.11448	-1.79852	-0.24645
N	1.43707	1.47546	0.27096
C	4.89527	-0.15960	0.38713
O	5.89277	-0.76318	0.40787
N	3.39065	0.91149	-1.52869
H	-1.19821	-1.61518	-0.30751
O	-0.62541	-4.08352	-0.49624
H	2.10663	-4.42059	-0.25825
H	3.69883	-2.58920	0.09457
C	-3.56632	2.27601	-0.34136
C	-3.07299	1.36441	-1.30555
C	-1.79318	0.82291	-1.17898
C	-1.45273	2.10303	0.85502
C	-2.74335	2.64284	0.74703
O	-4.82691	2.73659	-0.54725
H	-3.72260	1.10025	-2.15459
H	-1.42165	0.13199	-1.95217
H	-0.82984	2.38124	1.72187
H	-3.09900	3.33882	1.52074
H	1.18618	2.47323	0.32101
N	3.40502	1.00134	-2.65001
C	-0.22912	-5.44089	-0.56470
C	-5.38569	3.65277	0.38228

H	-5.46245	3.20809	1.40232
H	-6.40354	3.88416	0.00967
H	-4.79354	4.59639	0.43674
H	0.27355	-5.77564	0.37430
H	0.45303	-5.63243	-1.42759
H	-1.15994	-6.02735	-0.70385

$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	26.09	0.06155	YES	YES
8	a	34.83	0.55472	YES	YES
9	a	39.94	0.11211	YES	YES
10	a	55.02	1.41485	YES	YES
11	a	61.32	0.55432	YES	YES
12	a	75.96	0.09883	YES	YES
13	a	78.07	0.42937	YES	YES
14	a	85.25	1.28896	YES	YES
15	a	92.37	0.44046	YES	YES
16	a	92.49	0.04775	YES	YES
17	a	95.62	0.01563	YES	YES
18	a	99.40	0.34592	YES	YES
19	a	105.38	1.50621	YES	YES
20	a	131.29	1.88156	YES	YES
21	a	152.28	1.77738	YES	YES
22	a	179.39	0.91144	YES	YES
23	a	193.40	1.05336	YES	YES
24	a	211.01	0.73731	YES	YES
25	a	229.07	0.61321	YES	YES
26	a	245.85	0.58944	YES	YES
27	a	248.15	0.19175	YES	YES
28	a	249.62	1.30908	YES	YES
29	a	293.02	2.31278	YES	YES
30	a	319.77	4.81215	YES	YES
31	a	323.00	2.00777	YES	YES
32	a	353.55	1.44663	YES	YES
33	a	371.32	14.70453	YES	YES
34	a	395.56	0.20087	YES	YES
35	a	416.35	2.33749	YES	YES
36	a	416.57	4.07155	YES	YES
37	a	431.39	0.67885	YES	YES
38	a	436.08	0.86495	YES	YES
39	a	458.24	1.05642	YES	YES
40	a	470.38	0.73743	YES	YES
41	a	480.03	2.19379	YES	YES
42	a	488.46	8.58009	YES	YES
43	a	493.52	1.35659	YES	YES
44	a	508.25	4.87336	YES	YES
45	a	512.49	6.34115	YES	YES
46	a	536.14	24.04596	YES	YES
47	a	545.10	4.21738	YES	YES
48	a	551.20	5.95627	YES	YES
49	a	571.91	6.25813	YES	YES

50	a	579.60	17.21781	YES	YES

[**4**]

SCF Energy (au) BP86/SV(P)	-2351.9348114380
SCF Energy (au) PBE0/def2-TZVPP	-2351.561490343
Zero Point Energy (au)	0.3016435
Chemical potential (kJ mol^{-1})	641.24
Dispersion correction (au) PBE0/def2-TZVPP	-0.05282759
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-2351.5706161977

xyz coordinates
42

Mn	3.25273	0.70147	0.51255
C	3.10069	0.44875	2.26004
C	4.02486	2.34334	0.69608
O	4.51794	3.39281	0.84134
O	2.97753	0.27024	3.40897
C	0.37354	0.64751	0.06833
C	-1.00760	1.17227	-0.06176
C	0.75784	-0.76718	-0.05412
C	2.16247	-1.00488	0.14652
C	2.56686	-2.35176	0.05816
C	1.66496	-3.40905	-0.19609
C	0.28887	-3.14313	-0.35710
C	-0.16322	-1.80968	-0.28099
N	1.38216	1.44863	0.35290
C	4.81293	-0.18358	0.49547
O	5.81167	-0.79192	0.49016
H	-1.24431	-1.62625	-0.37976
O	-0.67154	-4.08952	-0.58070
H	2.04995	-4.43938	-0.24633
H	3.62773	-2.61818	0.20826
C	-3.61526	2.28365	-0.31171
C	-3.12169	1.37984	-1.28310
C	-1.84586	0.82929	-1.15462
C	-1.50982	2.08316	0.89530
C	-2.79619	2.63184	0.78588
O	-4.87111	2.75511	-0.52004
H	-3.76821	1.12847	-2.13838
H	-1.47724	0.14348	-1.93393
H	-0.89253	2.34554	1.77102
H	-3.15234	3.31986	1.56645
H	1.11756	2.43927	0.46199
O	3.26814	0.82544	-1.65675
C	-0.28082	-5.44963	-0.63199
C	-5.42994	3.66380	0.41730
H	-5.51607	3.20703	1.43112
H	-6.44373	3.90645	0.04098
H	-4.83175	4.60252	0.48696
H	0.18344	-5.78481	0.32613
H	0.43327	-5.64646	-1.46738
H	-1.20896	-6.03086	-0.80637
H	3.04944	-0.12522	-1.82427
H	2.42359	1.30173	-1.83651

$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	26.00	0.53254	YES	YES
8	a	35.02	0.48641	YES	YES
9	a	38.97	0.38077	YES	YES
10	a	55.92	2.07081	YES	YES
11	a	67.12	0.31764	YES	YES
12	a	74.09	0.11402	YES	YES
13	a	82.78	0.71109	YES	YES
14	a	86.65	1.60959	YES	YES
15	a	91.17	0.04151	YES	YES
16	a	97.47	2.32132	YES	YES
17	a	99.92	0.92330	YES	YES
18	a	121.20	1.55990	YES	YES
19	a	131.29	2.54849	YES	YES
20	a	148.42	2.18503	YES	YES
21	a	157.20	4.18466	YES	YES
22	a	185.88	8.59400	YES	YES
23	a	199.25	1.75080	YES	YES
24	a	210.12	24.35927	YES	YES
25	a	212.49	4.10185	YES	YES
26	a	236.29	5.26463	YES	YES
27	a	247.00	1.41147	YES	YES
28	a	247.72	3.29396	YES	YES
29	a	253.34	6.73868	YES	YES
30	a	296.62	2.35600	YES	YES
31	a	312.22	25.70654	YES	YES
32	a	322.85	2.81274	YES	YES
33	a	329.76	11.29843	YES	YES
34	a	353.46	2.99418	YES	YES
35	a	415.92	3.04308	YES	YES
36	a	424.94	4.92278	YES	YES
37	a	436.10	0.52141	YES	YES
38	a	457.50	1.80447	YES	YES
39	a	459.25	5.11155	YES	YES
40	a	472.75	8.95774	YES	YES
41	a	484.12	43.60404	YES	YES
42	a	490.47	0.95525	YES	YES
43	a	506.09	5.02604	YES	YES
44	a	509.17	2.50731	YES	YES
45	a	529.09	21.93988	YES	YES
46	a	537.94	33.26943	YES	YES
47	a	550.15	11.82123	YES	YES
48	a	556.60	159.65150	YES	YES
49	a	565.93	71.78882	YES	YES
50	a	573.73	15.89494	YES	YES

CO

SCF Energy (au) BP86/SV(P)	-113.230064069
SCF Energy (au) PBE0/def2-TZVPP	-113.2302273127
Zero Point Energy (au)	0.0049005
Chemical potential (kJ mol^{-1})	-37.48
Dispersion correction (au) PBE0/def2-TZVPP	-0.00033780
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-113.2305691586

xyz coordinates

2

C	0.00000	0.00000	0.57100
O	0.00000	0.00000	-0.57100

$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	a1	2151.08	60.66925	YES	YES

Heptane

SCF Energy (au) BP86/SV(P)	-276.1593180343
SCF Energy (au) PBE0/def2-TZVPP	-276.1417117921
Zero Point Energy (au)	0.2107137
Chemical potential (kJ mol^{-1})	460.98
Dispersion correction (au) PBE0/def2-TZVPP	-0.01471318
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-276.1422777983

xyz coordinates

23

C	1.85757	-2.97819	1.63815
C	0.56993	-2.26372	1.20650
H	1.63900	-3.94987	2.13420
H	2.44313	-2.35926	2.35518
H	2.51726	-3.18797	0.76559
H	-0.01093	-2.92617	0.52186
C	0.81746	-0.91437	0.51235
H	-0.08271	-2.10300	2.09740
H	1.39975	-0.25117	1.19652
C	-0.46820	-0.19163	0.07897
H	1.46922	-1.07473	-0.38057
C	-0.22099	1.15762	-0.61445
H	-1.11945	-0.03213	0.97222
H	-1.04980	-0.85536	-0.60502
H	0.35963	1.82229	0.06971
C	-1.50707	1.87992	-1.04890
H	0.43093	0.99926	-1.50761
C	-1.25220	3.22668	-1.73865
H	-2.15879	2.03659	-0.15662
H	-2.08621	1.21563	-1.73308
H	-0.70739	3.92897	-1.06756
H	-2.20394	3.71909	-2.03806
H	-0.63620	3.10151	-2.65813

$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	60.08	0.00058	YES	YES
8	a	69.76	0.00014	YES	YES
9	a	95.99	0.00884	YES	YES
10	a	139.13	0.00012	YES	YES
11	a	143.13	0.00039	YES	YES
12	a	238.45	0.00003	YES	YES
13	a	246.62	0.00004	YES	YES
14	a	249.00	0.00043	YES	YES
15	a	296.47	0.00453	YES	YES
16	a	407.81	0.06774	YES	YES
17	a	471.92	0.04358	YES	YES
18	a	723.56	6.01809	YES	YES
19	a	726.96	0.00072	YES	YES
20	a	757.44	1.98990	YES	YES
21	a	826.64	0.00149	YES	YES

22	a	868.53	2.28104	YES	YES
23	a	899.60	1.81290	YES	YES
24	a	914.56	1.20882	YES	YES
25	a	988.34	0.00259	YES	YES
26	a	997.82	0.00204	YES	YES
27	a	1031.91	0.02471	YES	YES
28	a	1050.27	1.01889	YES	YES
29	a	1056.90	0.71985	YES	YES
30	a	1064.84	1.96649	YES	YES
31	a	1128.20	1.07902	YES	YES
32	a	1167.12	0.19505	YES	YES
33	a	1202.04	0.00081	YES	YES
34	a	1215.84	5.81204	YES	YES
35	a	1253.59	0.02151	YES	YES
36	a	1276.36	0.00666	YES	YES
37	a	1282.53	0.00195	YES	YES
38	a	1290.96	0.02064	YES	YES
39	a	1297.10	0.76738	YES	YES
40	a	1328.57	2.83233	YES	YES
41	a	1359.14	0.61598	YES	YES
42	a	1364.29	2.60863	YES	YES
43	a	1366.82	1.55053	YES	YES
44	a	1370.36	0.09231	YES	YES
45	a	1423.54	0.31652	YES	YES
46	a	1424.09	0.04094	YES	YES
47	a	1428.46	0.03606	YES	YES
48	a	1433.58	1.23573	YES	YES
49	a	1436.43	7.96972	YES	YES
50	a	1437.71	9.02038	YES	YES

N_2

SCF Energy (au) BP86/SV(P)	-109.4489525196
SCF Energy (au) PBE0/def2-TZVPP	-109.4449257462
Zero Point Energy (au)	0.0054354
Chemical potential (kJ mol^{-1})	-34.28
Dispersion correction (au) PBE0/def2-TZVPP	-0.00035163
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-109.4451555170

xyz coordinates
2

N	0.00000	0.00000	0.55600
N	0.00000	0.00000	-0.55600

$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	a1g	2385.86	0.00000	NO	YES

H_2O

SCF Energy (au) BP86/SV(P)	-76.3451982082
SCF Energy (au) PBE0/def2-TZVPP	-76.379976764
Zero Point Energy (au)	0.0199812
Chemical potential (kJ mol^{-1})	5.89
Dispersion correction (au) PBE0/def2-TZVPP	-0.00027693
SCF Energy (au) PBE0/def2-TZVPP COSMO (Heptane)	-76.3840924503

xyz coordinates

$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	a1	1604.23	61.98164	YES	YES
8	a1	3526.13	0.10543	YES	YES
9	b1	3640.35	16.43822	YES	YES