

-Supporting Information-

Manganese-complex catalyzed dehydrogenation of formic acid to CO₂ and H₂. A theoretical investigation on a green and sustainable route

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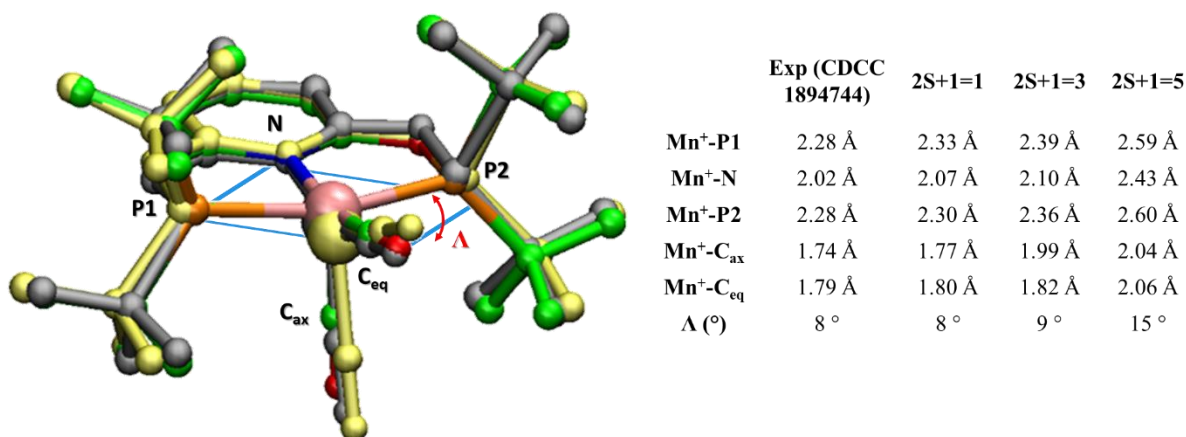


Figure S1. On the left, superposition of substrate-free complex fixing singlet, triplet (green) and quintet (gray) state. On the right, comparison between optimized and experimental observed relevant geometrical parameters.

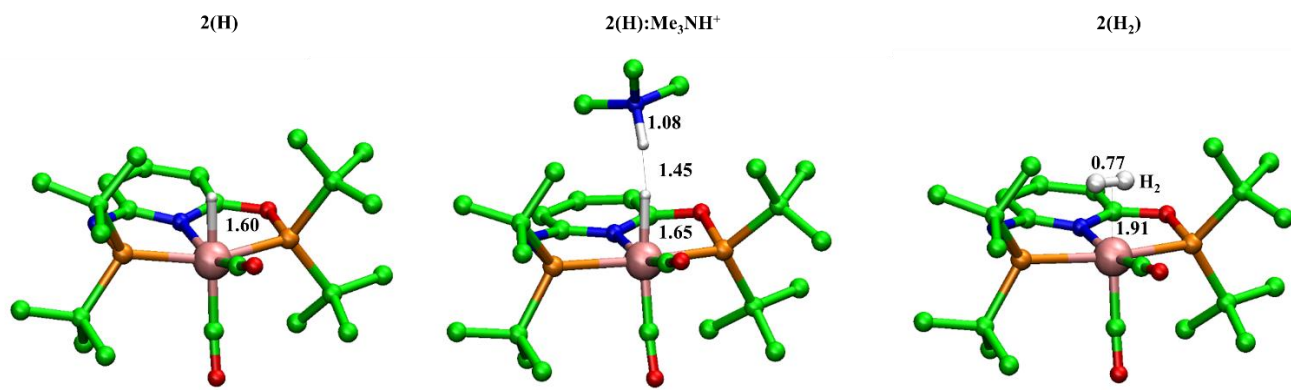


Figure S2. B3LYP-D3/6-31+G(d,p) optimized geometries of **2(H)**, **2(H):Me₃NH⁺** and **2(H₂)** stationary points. Relevant distances (in black) are in Å.

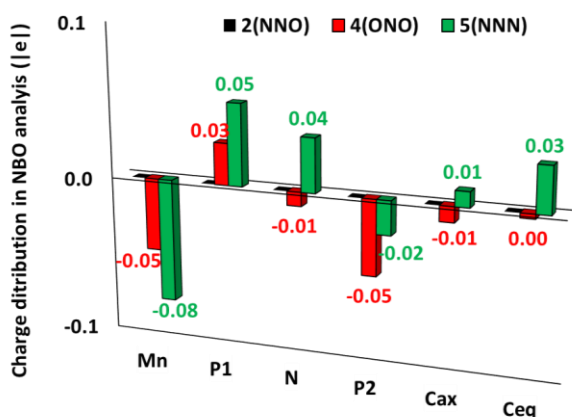


Figure S3. Charge distribution in NBO population of relevant atoms.

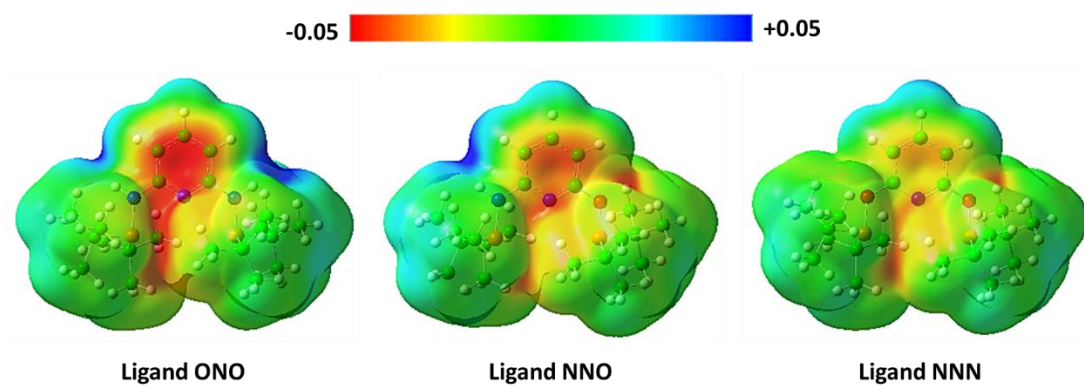


Figure S4. Map of electrostatic potential plotted for the three different ligands.

	$\langle S_z \rangle$	$\langle S^2 \rangle$	S.C.	S.C (%)
$2S+1=3$	1.000	2.107	0.049	4.9
$2S+1=5$	2.000	6.292	0.054	5.4

$$\text{S. C.} = \frac{S^2 - S_z(S_z + 1)}{S_z(S_z + 1)}$$

Table S1. Calculated spin contamination for triplet and quintet spin states.

Cartesian coordinates

Complex 2 ($2S+1=1$)

Mn	0.004	-0.461	0.085	C	-1.244	2.266	0.204	C	-1.352	3.647	0.318
N	-0.055	1.609	0.137	C	1.092	2.354	0.151	C	1.063	3.751	0.264

C	-0.17	4.387	0.353	H	-1.47	1.148	-2.511	P	2.338	-0.032	-0.082
H	-2.333	4.103	0.371	C	1.857	-0.111	-2.758	P	-2.294	-0.122	-0.144
H	1.99	4.313	0.279	H	1.071	-0.864	-2.651	N	2.29	1.58	0.55
H	-0.213	5.468	0.443	H	1.418	0.883	-2.612	H	3.132	2.131	0.658
C	0.037	-2.207	-0.373	H	2.216	-0.164	-3.793	O	-2.353	1.55	0.193
C	0.009	-0.922	1.791	C	3.448	-1.861	-1.92	C	2.971	0.198	-1.857
O	0.056	-3.322	-0.688	H	2.649	-2.549	-1.625	C	3.58	-0.921	1.044
O	0.014	-1.25	2.905	H	3.686	-2.068	-2.971	C	-3.014	-0.151	-1.889
P	2.3	-0.071	-0.06	H	4.34	-2.093	-1.333	C	-3.489	-0.756	1.176
P	-2.271	-0.153	-0.05	C	4.191	0.553	-2.158	C	-4.953	-0.347	0.933
N	2.273	1.661	0.032	H	5.066	0.429	-1.519	H	-5.383	-0.833	0.054
H	3.12	2.213	0.036	H	4.506	0.33	-3.184	H	-5.548	-0.658	1.8
O	-2.38	1.543	0.145	H	3.887	1.606	-2.14	H	-5.062	0.737	0.828
C	3.026	-0.384	-1.788	C	3.104	0.237	2.588	C	-3.368	-2.294	1.235
C	3.487	-0.578	1.332	H	2.049	0.158	2.849	H	-4.002	-2.665	2.049
C	-2.957	-0.322	-1.803	H	3.681	-0.146	3.438	H	-3.703	-2.777	0.313
C	-3.469	-0.735	1.285	H	3.348	1.298	2.474	H	-2.345	-2.624	1.437
C	-4.952	-0.515	0.936	C	3.281	-2.085	1.602	C	-3.031	-0.138	2.518
H	-5.28	-1.129	0.094	H	3.934	-2.388	2.429	H	-3.197	0.943	2.539
H	-5.556	-0.806	1.804	H	2.253	-2.314	1.892	H	-3.618	-0.587	3.327
H	-5.172	0.534	0.719	H	3.538	-2.705	0.738	H	-1.977	-0.325	2.738
C	-3.199	-2.24	1.511	C	4.97	-0.302	1.018	C	-4.145	0.875	-2.096
H	-3.87	-2.602	2.298	H	5.161	0.753	0.791	H	-4.423	0.867	-3.157
H	-3.391	-2.838	0.614	H	5.564	-0.549	1.907	H	-5.043	0.643	-1.522
H	-2.174	-2.433	1.836	H	5.35	-0.911	0.195	H	-3.823	1.889	-1.841
C	-3.153	0.067	2.569	Complex 2 (2S+1=3)				C	-3.493	-1.58	-2.214
H	-3.423	1.12	2.456	Mn	0.014	-0.529	0.175	H	-4.39	-1.856	-1.654
H	-3.748	-0.351	3.39	N	-0.043	1.544	0.489	H	-3.745	-1.63	-3.28
H	-2.105	0.009	2.868	C	-1.221	2.217	0.503	H	-2.718	-2.333	-2.028
C	-4.175	0.576	-2.094	C	1.101	2.262	0.693	C	-1.841	0.21	-2.825
H	-4.386	0.533	-3.17	C	-1.332	3.571	0.804	H	-1.052	-0.545	-2.78
H	-5.076	0.253	-1.574	C	1.073	3.627	1.011	H	-2.206	0.252	-3.858
H	-3.979	1.62	-1.833	C	-0.158	4.271	1.076	H	-1.407	1.187	-2.587
C	-3.278	-1.804	-2.08	H	-2.309	4.036	0.809	C	1.779	0.808	-2.626
H	-4.144	-2.155	-1.511	H	1.999	4.162	1.186	H	0.922	0.132	-2.631
H	-3.517	-1.922	-3.144	H	-0.202	5.328	1.32	H	1.46	1.767	-2.202
H	-2.43	-2.463	-1.861	C	0.049	-2.149	-0.655	H	2.074	0.986	-3.667
C	-1.796	0.123	-2.719	C	0.041	-1.521	1.897	C	3.309	-1.179	-2.461
H	-0.934	-0.545	-2.628	O	0.067	-3.166	-1.215	H	2.486	-1.894	-2.345
H	-2.12	0.086	-3.766	O	0.052	-2.237	2.796	H	3.492	-1.061	-3.536

H	4.211	-1.617	-2.024	C	-3.704	-0.668	1.204	H	3.172	1.124	2.641
C	4.167	1.161	-1.979	C	-5.14	-0.171	0.97	C	3.664	-2.084	1.365
H	5.075	0.79	-1.502	H	-5.59	-0.618	0.079	H	4.272	-2.409	2.217
H	4.393	1.299	-3.043	H	-5.759	-0.46	1.828	H	2.651	-2.473	1.516
H	3.936	2.153	-1.574	H	-5.184	0.919	0.878	H	4.077	-2.555	0.469
C	3.262	-0.52	2.501	C	-3.663	-2.213	1.219	C	5.123	-0.036	1.111
H	2.212	-0.666	2.766	H	-4.312	-2.577	2.024	H	5.173	1.054	0.996
H	3.861	-1.146	3.173	H	-4.022	-2.653	0.285	H	5.705	-0.293	2.004
H	3.514	0.526	2.701	H	-2.654	-2.596	1.41	H	5.62	-0.498	0.254
C	3.367	-2.44	0.863	C	-3.195	-0.128	2.56	2:FA			
H	4.058	-2.976	1.524	H	-3.267	0.962	2.613	Mn	-0.011	-0.562	0.27
H	2.351	-2.748	1.125	H	-3.812	-0.551	3.362	N	0.033	1.324	-0.753
H	3.566	-2.774	-0.159	H	-2.156	-0.413	2.762	C	1.212	1.937	-0.98
C	5.051	-0.565	0.757	C	-4.217	1.009	-2.057	C	-1.098	2.063	-0.871
H	5.242	0.512	0.825	H	-4.426	1.08	-3.132	C	1.319	3.21	-1.537
H	5.681	-1.052	1.511	H	-5.149	0.736	-1.56	C	-1.085	3.354	-1.412
H	5.385	-0.918	-0.221	H	-3.916	2.001	-1.708	C	0.141	3.913	-1.763
Complex 2 (2S+1=5)				C	-3.573	-1.437	-2.261	H	2.299	3.631	-1.718
Mn	0.036	-0.823	0.224	H	-4.493	-1.73	-1.748	H	-2.012	3.907	-1.52
N	-0.055	1.605	0.276	H	-3.784	-1.436	-3.337	H	0.178	4.915	-2.178
C	-1.226	2.252	0.405	H	-2.814	-2.208	-2.08	C	0	-1.876	1.493
C	1.084	2.334	0.356	C	-1.876	0.378	-2.694	C	-0.052	-1.81	-0.978
C	-1.342	3.618	0.65	H	-1.057	-0.345	-2.607	O	0.016	-2.71	2.302
C	1.069	3.717	0.601	H	-2.169	0.424	-3.75	O	-0.1	-2.717	-1.717
C	-0.16	4.35	0.753	H	-1.491	1.364	-2.412	P	-2.353	-0.177	0.043
H	-2.323	4.066	0.746	C	2.022	0.179	-2.762	P	2.275	-0.275	0.007
H	1.999	4.271	0.666	H	1.25	-0.593	-2.682	N	-2.265	1.496	-0.401
H	-0.198	5.418	0.945	H	1.559	1.151	-2.554	H	-3.106	2.026	-0.585
C	0.006	-2.496	-0.979	H	2.373	0.192	-3.801	O	2.35	1.29	-0.669
C	0.002	-1.812	2.007	C	3.746	-1.528	-2.09	C	-3.585	-0.178	1.503
O	-0.028	-3.414	-1.669	H	3.004	-2.301	-1.853	C	-3.245	-0.869	-1.51
O	-0.025	-2.377	3.009	H	3.988	-1.626	-3.155	C	3.475	-0.15	1.476
P	2.479	-0.021	-0.078	H	4.659	-1.742	-1.527	C	3.163	-1.127	-1.453
P	-2.448	-0.1	-0.075	C	4.314	0.938	-2.089	C	4.61	-0.64	-1.655
N	2.288	1.675	0.17	H	5.195	0.802	-1.459	H	5.285	-0.964	-0.861
H	3.108	2.266	0.22	H	4.641	0.847	-3.132	H	4.988	-1.062	-2.595
O	-2.388	1.557	0.278	H	3.942	1.961	-1.96	H	4.659	0.449	-1.736
C	3.215	-0.107	-1.822	C	3.102	0.032	2.603	C	3.155	-2.659	-1.285
C	3.681	-0.541	1.29	H	2.052	-0.241	2.751				
C	-3.101	-0.03	-1.843	H	3.671	-0.372	3.448				

H	3.529	-3.116	-2.21	H	-2.371	-2.875	-1.237	H	5.317	0.104	-1.33
H	3.806	-2.988	-0.473	H	-4.068	-2.766	-0.758	C	2.833	-2.236	-1.909
H	2.158	-3.06	-1.106	C	-4.659	-0.3	-1.73	H	3.444	-2.69	-2.698
C	2.396	-0.733	-2.737	H	-4.668	0.796	-1.756	H	2.927	-2.861	-1.014
H	2.53	0.327	-2.964	H	-5.025	-0.643	-2.706	H	1.795	-2.269	-2.235
H	2.805	-1.312	-3.574	H	-5.377	-0.635	-0.979	C	3.099	0.098	-2.892
H	1.328	-0.938	-2.691	O	-0.226	0.81	1.919	H	3.563	1.079	-2.756
C	4.529	0.953	1.279	C	0.071	2.036	2.148	H	3.566	-0.386	-3.759
H	5.143	1.006	2.187	O	0.963	2.727	1.637	H	2.048	0.249	-3.127
H	5.195	0.771	0.436	H	-0.572	2.498	2.932	C	4.741	0.707	1.163
H	4.047	1.924	1.14	TS rot				H	5.081	1.074	2.139
C	4.134	-1.525	1.704	Mn	-0.006	-0.525	-0.194	H	5.507	0.028	0.793
H	4.844	-1.798	0.922	N	0.038	1.537	0.099	H	4.673	1.572	0.494
H	4.686	-1.486	2.65	C	1.164	2.238	-0.158	C	3.547	-1.388	1.96
H	3.39	-2.325	1.797	C	-1.053	2.196	0.568	H	4.075	-2.053	1.266
C	2.675	0.191	2.747	C	1.254	3.618	0.013	H	4.154	-1.318	2.872
H	1.857	-0.509	2.927	C	-1.028	3.576	0.811	H	2.583	-1.834	2.221
H	3.364	0.144	3.6	C	0.135	4.28	0.517	C	2.606	0.941	2.352
H	2.266	1.197	2.688	H	2.183	4.124	-0.213	H	1.554	0.705	2.468
C	-2.825	0.001	2.831	H	-1.908	4.074	1.203	H	3.059	0.837	3.345
H	-2.072	-0.774	2.982	H	0.173	5.351	0.686	H	2.696	1.989	2.052
H	-2.316	0.96	2.884	C	-0.034	-2.348	-0.147	C	-2.814	-1.746	2.179
H	-3.558	-0.062	3.646	C	-0.026	-0.571	-1.938	H	-2.012	-2.397	1.828
C	-4.297	-1.542	1.568	O	-0.081	-3.502	-0.199	H	-2.391	-1.031	2.885
H	-3.583	-2.373	1.569	O	-0.05	-0.682	-3.103	H	-3.535	-2.363	2.73
H	-4.86	-1.594	2.508	P	-2.329	-0.1	-0.061	C	-4.24	-2.145	0.184
H	-5.008	-1.694	0.754	P	2.311	-0.126	-0.197	H	-3.503	-2.771	-0.332
C	-4.612	0.965	1.402	N	-2.185	1.433	0.764	H	-4.809	-2.799	0.855
H	-5.212	0.935	0.491	H	-3.01	1.952	1.037	H	-4.938	-1.747	-0.555
H	-5.302	0.893	2.251	O	2.25	1.562	-0.581	C	-4.626	-0.135	1.679
H	-4.119	1.94	1.47	C	-3.567	-1.05	1.033	H	-5.234	0.418	0.962
C	-2.401	-0.425	-2.728	C	-3.225	0.442	-1.673	H	-5.305	-0.761	2.27
H	-1.355	-0.718	-2.659	C	3.372	0.025	1.374	H	-4.163	0.572	2.376
H	-2.818	-0.893	-3.627	C	3.338	-0.797	-1.659	C	-2.405	1.603	-2.28
H	-2.438	0.659	-2.868	C	4.86	-0.879	-1.457	H	-1.354	1.363	-2.426
C	-3.326	-2.408	-1.474	H	5.141	-1.517	-0.616	H	-2.828	1.846	-3.262
H	-3.627	-2.77	-2.465	H	5.289	-1.326	-2.362	H	-2.466	2.504	-1.664

C	-3.286	-0.726	-2.679	H	5.279	-1.416	-0.193	H	-2.699	-3.202	-2.157
H	-3.648	-0.341	-3.64	H	4.908	-2.474	-1.551	H	-2.381	-1.524	-2.627
H	-2.312	-1.179	-2.859	H	4.642	-0.732	-1.708	C	-3.22	-2.896	0.47
H	-3.974	-1.51	-2.361	C	3.169	-2.916	0.555	H	-3.474	-3.842	-0.023
C	-4.647	0.985	-1.45	H	3.495	-3.851	0.081	H	-2.274	-3.047	0.988
H	-4.668	1.808	-0.727	H	3.881	-2.691	1.351	H	-3.99	-2.703	1.219
H	-5.017	1.387	-2.402	H	2.198	-3.105	1.009	C	-4.59	-1.549	-1.123
H	-5.353	0.218	-1.126	C	2.318	-2.265	-1.745	H	-4.64	-0.741	-1.861
O	0.476	-1.873	2.228	H	2.434	-1.564	-2.577	H	-4.926	-2.464	-1.628
C	-0.024	-0.82	2.717	H	2.693	-3.241	-2.072	H	-5.303	-1.341	-0.323
O	-0.138	-0.441	3.886	H	1.253	-2.373	-1.54	O	-0.015	3.196	-0.408
H	-0.445	-0.097	1.937	C	4.706	1.328	0.41	C	-0.025	2.799	0.751
2:FA'				H	5.248	2.015	1.071	O	-0.041	3.239	1.889
Mn	-0.002	-0.281	0.502	H	5.411	0.57	0.075	H	-0.014	1.508	0.788
N	0.052	0.541	-1.433	H	4.367	1.899	-0.458	TS1			
C	1.224	0.94	-1.972	C	3.996	-0.145	2.352	Mn	-0.003	0.32	-0.522
C	-1.087	0.997	-2.019	H	4.689	-0.919	2.014	N	0.05	-0.498	1.462
C	1.331	1.633	-3.173	H	4.525	0.477	3.083	C	1.223	-0.874	2.008
C	-1.075	1.688	-3.238	H	3.162	-0.626	2.877	C	-1.089	-0.929	2.06
C	0.149	1.996	-3.814	C	2.748	1.947	1.792	C	1.331	-1.532	3.231
H	2.31	1.898	-3.548	H	1.873	1.655	2.372	C	-1.078	-1.585	3.299
H	-2.009	2.009	-3.685	H	3.425	2.495	2.46	C	0.149	-1.874	3.883
H	0.186	2.546	-4.749	H	2.427	2.641	1.013	H	2.31	-1.782	3.618
C	-0.021	-0.363	2.289	C	-2.796	1.889	1.863	H	-2.011	-1.89	3.758
C	-0.017	-2.046	0.446	H	-1.944	1.549	2.45	H	0.186	-2.392	4.837
O	-0.028	-0.379	3.45	H	-2.437	2.621	1.138	C	-0.021	0.346	-2.301
O	-0.033	-3.213	0.528	H	-3.487	2.407	2.54	C	-0.02	2.092	-0.456
P	-2.316	-0.199	0.084	C	-4.094	-0.206	2.259	O	-0.028	0.299	-3.465
P	2.291	-0.234	0.141	H	-3.287	-0.739	2.774	O	-0.037	3.26	-0.545
N	-2.264	0.76	-1.351	H	-4.627	0.386	3.012	P	-2.302	0.21	-0.092
H	-3.106	1.06	-1.822	H	-4.798	-0.941	1.86	P	2.274	0.246	-0.15
O	2.367	0.656	-1.312	C	-4.715	1.386	0.391	N	-2.262	-0.713	1.374
C	-3.555	0.745	1.176	H	-5.349	0.671	-0.131	H	-3.11	-0.967	1.862
C	-3.163	-1.782	-0.595	H	-5.349	1.931	1.101	O	2.361	-0.61	1.331
C	3.514	0.755	1.199	H	-4.345	2.125	-0.328	C	-3.524	-0.781	-1.165
C	3.141	-1.809	-0.518	C	-2.314	-2.239	-1.802	C	-3.183	1.795	0.537
C	4.578	-1.575	-1.015	H	-1.26	-2.372	-1.563	C	3.486	-0.785	-1.185

C	3.156	1.825	0.461	C	-2.358	2.292	1.745	C	-3.392	-0.512	-1.385
C	4.6	1.598	0.939	H	-1.299	2.417	1.522	C	3.143	-0.379	1.727
H	5.286	1.415	0.109	H	-2.749	3.266	2.061	C	3.36	-0.615	-1.368
H	4.943	2.51	1.445	H	-2.443	1.605	2.593	C	4.847	-0.27	-1.193
H	4.673	0.773	1.652	C	-3.227	2.879	-0.56	H	5.332	-0.872	-0.421
C	3.169	2.903	-0.642	H	-3.483	3.841	-0.098	H	5.364	-0.479	-2.139
H	3.503	3.85	-0.201	H	-2.275	3.01	-1.072	H	4.995	0.789	-0.964
H	3.866	2.652	-1.444	H	-3.99	2.665	-1.31	C	3.218	-2.126	-1.635
H	2.19	3.079	-1.084	C	-4.618	1.572	1.047	H	3.782	-2.381	-2.541
C	2.357	2.319	1.689	H	-4.68	0.779	1.802	H	3.622	-2.727	-0.815
H	2.487	1.642	2.539	H	-4.964	2.496	1.527	H	2.181	-2.422	-1.793
H	2.741	3.303	1.982	H	-5.319	1.346	0.241	C	2.855	0.186	-2.588
H	1.289	2.424	1.501	O	0.003	-3.256	0.528	H	3.081	1.25	-2.477
C	4.688	-1.335	-0.395	C	-0.016	-3.081	-0.653	H	3.369	-0.182	-3.484
H	5.212	-2.057	-1.033	O	-0.035	-3.456	-1.785	H	1.784	0.078	-2.757
H	5.407	-0.569	-0.111	H	-0.016	-1.421	-0.811	C	4.33	0.588	1.897
H	4.363	-1.859	0.507	2(H)				H	4.742	0.455	2.906
C	3.953	0.072	-2.376	Mn	-0.01	-0.591	-0.068	H	5.137	0.414	1.189
H	4.65	0.857	-2.075	N	0.057	1.687	-0.224	H	4.006	1.628	1.799
H	4.473	-0.574	-3.093	C	1.239	2.313	-0.164	C	3.606	-1.845	1.829
H	3.111	0.535	-2.905	C	-1.087	2.397	-0.147	H	4.412	-2.076	1.128
C	2.713	-1.996	-1.727	C	1.354	3.705	-0.173	H	3.986	-2.03	2.842
H	1.828	-1.718	-2.298	C	-1.07	3.802	-0.162	H	2.782	-2.545	1.654
H	3.379	-2.569	-2.385	C	0.168	4.441	-0.191	C	2.165	-0.101	2.885
H	2.407	-2.658	-0.914	H	2.331	4.168	-0.146	H	1.348	-0.823	2.912
C	-2.753	-1.952	-1.789	H	-1.996	4.364	-0.126	H	2.724	-0.165	3.827
H	-1.886	-1.633	-2.367	H	0.21	5.526	-0.199	H	1.723	0.898	2.816
H	-2.414	-2.648	-1.021	C	-0.042	-2.204	0.653	C	-2.205	-0.179	2.891
H	-3.429	-2.5	-2.457	C	-0.02	-1.187	-1.759	H	-1.426	-0.941	2.894
C	-4.04	0.127	-2.296	O	-0.064	-3.233	1.212	H	-1.714	0.798	2.859
H	-3.221	0.645	-2.809	O	-0.032	-1.694	-2.817	H	-2.772	-0.251	3.829
H	-4.552	-0.493	-3.041	P	-2.237	-0.086	0.082	C	-3.704	-1.817	1.753
H	-4.754	0.872	-1.94	P	2.209	-0.165	0.081	H	-2.907	-2.533	1.528
C	-4.701	-1.393	-0.383	N	-2.241	1.662	-0.018	H	-4.075	-2.042	2.76
H	-5.353	-0.658	0.088	H	-3.104	2.187	0.006	H	-4.528	-1.984	1.055
H	-5.314	-1.974	-1.083	O	2.349	1.557	-0.068	C	-4.343	0.627	1.941
H	-4.348	-2.094	0.381	C	-3.187	-0.367	1.719	H	-5.105	0.597	1.163

H	-4.836	0.384	2.89	C	-3.37	0.15	-1.485	H	4.163	2.205	0.276
H	-3.97	1.653	2.029	C	-3.037	-2.032	0.691	C	2.778	-2.266	1.802
C	-2.856	0.272	-2.602	C	-4.49	-1.722	1.094	H	1.701	-2.411	1.739
H	-1.784	0.146	-2.751	H	-5.166	-1.682	0.238	H	3.225	-3.234	2.055
H	-3.362	-0.091	-3.505	H	-4.846	-2.53	1.745	H	2.978	-1.583	2.633
H	-3.06	1.343	-2.508	H	-4.569	-0.787	1.655	C	3.418	-2.874	-0.576
C	-3.292	-2.025	-1.662	C	-3.009	-3.314	-0.168	H	3.926	-3.754	-0.163
H	-3.852	-2.259	-2.575	H	-3.343	-4.152	0.456	H	2.415	-3.184	-0.865
H	-2.261	-2.346	-1.813	H	-3.687	-3.256	-1.02	H	3.957	-2.58	-1.478
H	-3.718	-2.621	-0.851	H	-2.014	-3.563	-0.535	C	4.881	-1.408	0.826
C	-4.873	-0.132	-1.223	C	-2.255	-2.273	2.005	H	4.967	-0.584	1.544
H	-5.009	0.936	-1.013	H	-2.409	-1.459	2.718	H	5.343	-2.285	1.296
H	-5.392	-0.339	-2.167	H	-2.636	-3.19	2.466	H	5.474	-1.166	-0.057
H	-5.375	-0.708	-0.443	H	-1.183	-2.405	1.857	H	-0.078	0.999	-1.01
H	-0.019	-0.156	1.473	C	-4.508	0.969	-0.849	C	-2.008	3.669	0.07
2(H):Me₃NH⁺				H	-5.105	1.419	-1.652	H	-2.309	2.994	0.867
Mn	0.092	-0.554	-0.489	H	-5.178	0.364	-0.24	H	-2.05	4.705	0.415
N	-0.022	0.426	1.356	H	-4.127	1.775	-0.219	H	-2.664	3.542	-0.789
C	-1.225	0.77	1.861	C	-3.951	-0.991	-2.346	C	-0.235	4.112	-1.563
C	1.095	0.798	2.033	H	-4.685	-1.591	-1.807	H	-0.42	5.177	-1.4
C	-1.387	1.367	3.111	H	-4.46	-0.549	-3.21	H	0.816	3.943	-1.788
C	1.021	1.358	3.32	H	-3.17	-1.655	-2.733	H	-0.848	3.752	-2.39
C	-0.233	1.626	3.856	C	-2.583	1.062	-2.447	C	0.313	3.677	0.797
H	-2.382	1.58	3.48	H	-1.835	0.512	-3.018	H	-0.081	3.247	1.711
H	1.93	1.59	3.864	H	-3.291	1.512	-3.154	H	1.308	3.291	0.588
H	-0.317	2.055	4.85	H	-2.066	1.865	-1.926	H	0.353	4.737	0.925
C	0.2	-0.879	-2.236	C	2.525	1.867	-1.881	N	-0.602	3.363	-0.326
C	0.195	-2.299	-0.108	H	1.711	1.426	-2.457	H	-0.488	2.316	-0.554
O	0.284	-1.008	-3.39	H	2.089	2.498	-1.104	TS2			
O	0.237	-3.46	0.01	H	3.123	2.506	-2.542	Mn	0.078	-0.482	-0.523
P	2.363	-0.282	-0.116	C	4.015	-0.056	-2.39	N	-0.027	0.374	1.388
P	-2.167	-0.59	-0.207	H	3.24	-0.657	-2.878	C	-1.227	0.716	1.903
N	2.284	0.651	1.363	H	4.446	0.603	-3.152	C	1.093	0.714	2.075
H	3.118	0.826	1.91	H	4.81	-0.722	-2.051	C	-1.382	1.284	3.167
O	-2.318	0.555	1.096	C	4.565	1.565	-0.518	C	1.026	1.243	3.375
C	3.441	0.808	-1.251	H	5.322	0.912	-0.086	C	-0.225	1.515	3.916
C	3.419	-1.758	0.489	H	5.072	2.221	-1.235	H	-2.374	1.504	3.538

H	1.937	1.455	3.923	H	-3.363	1.661	-3.04	H	1.376	3.275	0.653
H	-0.303	1.926	4.917	H	-2.009	1.844	-1.912	H	0.384	4.691	0.989
C	0.188	-0.695	-2.291	C	2.601	1.902	-1.793	N	-0.514	3.332	-0.311
C	0.163	-2.248	-0.304	H	1.811	1.487	-2.422	H	-0.345	2.149	-0.597
O	0.28	-0.765	-3.448	H	2.135	2.499	-1.01	2(H₂)			
O	0.189	-3.413	-0.294	H	3.223	2.567	-2.405	Mn	0.006	-0.52	-0.048
P	2.366	-0.295	-0.109	C	4.094	-0.013	-2.323	N	-0.048	1.594	-0.255
P	-2.194	-0.557	-0.208	H	3.332	-0.59	-2.858	C	-1.23	2.237	-0.386
N	2.285	0.562	1.409	H	4.551	0.672	-3.048	C	1.098	2.309	-0.41
H	3.118	0.72	1.961	H	4.875	-0.696	-1.986	C	-1.337	3.614	-0.545
O	-2.325	0.525	1.141	C	4.594	1.532	-0.375	C	1.079	3.701	-0.564
C	3.49	0.815	-1.174	H	5.306	0.852	0.092	C	-0.151	4.347	-0.616
C	3.366	-1.835	0.437	H	5.159	2.176	-1.058	H	-2.314	4.071	-0.623
C	-3.423	0.22	-1.436	H	4.17	2.179	0.401	H	2.009	4.251	-0.659
C	-3.026	-2.044	0.653	C	2.673	-2.413	1.693	H	-0.19	5.424	-0.734
C	-4.456	-1.735	1.133	H	1.609	-2.604	1.562	C	0.032	-2.31	-0.264
H	-5.167	-1.636	0.31	H	3.147	-3.369	1.938	C	0.016	-0.788	1.713
H	-4.798	-2.572	1.754	H	2.794	-1.753	2.557	O	0.046	-3.456	-0.43
H	-4.495	-0.83	1.747	C	3.388	-2.886	-0.692	O	0.028	-1.055	2.842
C	-3.053	-3.285	-0.264	H	3.843	-3.806	-0.305	P	2.334	-0.108	-0.092
H	-3.355	-4.15	0.339	H	2.394	-3.145	-1.054	P	-2.304	-0.178	-0.077
H	-3.778	-3.187	-1.072	H	3.987	-2.561	-1.543	N	2.271	1.587	-0.455
H	-2.082	-3.52	-0.699	C	4.82	-1.527	0.845	H	3.12	2.135	-0.515
C	-2.191	-2.356	1.918	H	4.89	-0.76	1.624	O	-2.362	1.5	-0.396
H	-2.28	-1.565	2.666	H	5.259	-2.441	1.262	C	3.4	-0.806	-1.509
H	-2.584	-3.276	2.366	H	5.444	-1.228	0.001	C	3.318	-0.115	1.54
H	-1.133	-2.522	1.714	H	-0.097	1.175	-0.911	C	-3.361	-0.835	-1.511
C	-4.513	1.055	-0.739	C	-1.917	3.629	0.065	C	-3.287	-0.182	1.543
H	-5.159	1.495	-1.508	H	-2.243	2.93	0.833	C	-4.769	0.2	1.378
H	-5.142	0.46	-0.078	H	-1.978	4.654	0.449	H	-5.347	-0.561	0.851
H	-4.089	1.868	-0.147	H	-2.563	3.538	-0.807	H	-5.204	0.3	2.38
C	-4.071	-0.888	-2.29	C	-0.134	4.116	-1.511	H	-4.891	1.16	0.869
H	-4.809	-1.471	-1.739	H	-0.343	5.178	-1.342	C	-3.196	-1.576	2.199
H	-4.592	-0.412	-3.13	H	0.925	3.981	-1.719	H	-3.696	-1.531	3.174
H	-3.328	-1.57	-2.715	H	-0.715	3.765	-2.367	H	-3.703	-2.342	1.608
C	-2.643	1.118	-2.417	C	0.366	3.634	0.835	H	-2.172	-1.904	2.377
H	-2.001	0.533	-3.078	H	-0.042	3.183	1.734	C	-2.65	0.897	2.449

H	-2.877	1.9	2.08	H	-2.033	-0.043	-3.08	H	1.584	0.83	2.561
H	-3.081	0.801	3.452	C	2.516	-0.999	-2.755	H	3.097	0.847	3.459
H	-1.569	0.809	2.554	H	1.74	-1.754	-2.604	H	2.863	1.956	2.102
C	-4.516	0.114	-1.887	H	2.055	-0.061	-3.084	C	3.253	-1.513	2.188
H	-5.027	-0.302	-2.762	H	3.15	-1.348	-3.578	H	3.725	-1.462	3.176
H	-5.255	0.227	-1.097	C	3.943	-2.185	-1.09	H	2.234	-1.87	2.336
H	-4.144	1.107	-2.155	H	3.149	-2.846	-0.724	H	3.795	-2.261	1.607
C	-3.888	-2.23	-1.12	H	4.392	-2.668	-1.965	C	4.796	0.289	1.384
H	-4.648	-2.185	-0.338	H	4.717	-2.116	-0.324	H	4.917	1.264	0.899
H	-4.35	-2.69	-2.001	C	4.548	0.138	-1.916	H	5.232	0.377	2.386
H	-3.085	-2.898	-0.788	H	5.246	0.353	-1.108	H	5.385	-0.45	0.839
C	-2.476	-0.994	-2.762	H	5.119	-0.339	-2.721	H	0.403	-0.284	-1.922
H	-1.688	-1.74	-2.626	H	4.166	1.084	-2.314	H	-0.365	-0.318	-1.934
H	-3.108	-1.34	-3.587	C	2.662	0.941	2.458				