

# Supplementary Information

## **Steric Effects of Alcohols on the [Mn<sub>4</sub>O<sub>4</sub>] Cubane-Type Structures**

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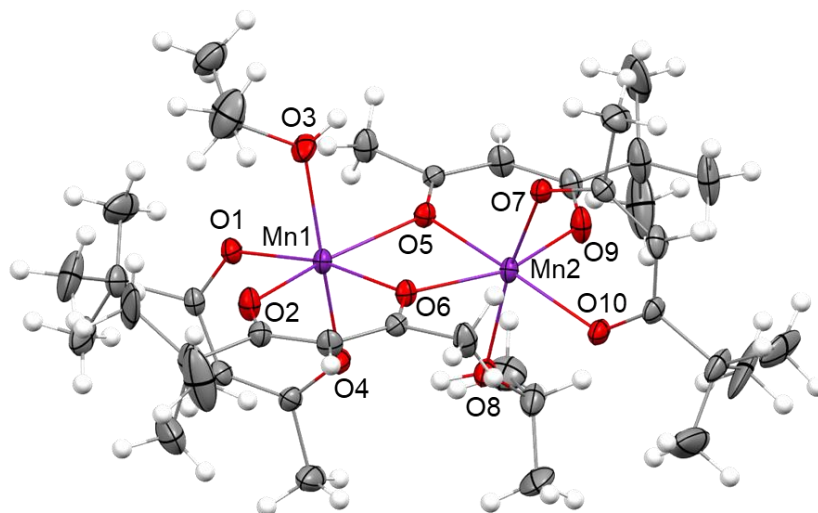
## Crystal Growth

Block-shaped yellow crystals of  $\text{Mn}_2(\text{dhd})_4(\text{iPrOH})_2$  (**1**),  $\text{Mn}_4(\text{dhd})_4(\text{OEt})_4(\text{EtOH})_4$  (**2**),  $\text{Mn}_4(\text{dhd})_6(\text{OMe})_2(\text{MeOH})_2$  (**3**) suitable for X-ray single crystal structural measurements were obtained by a cooling method, whereby *i*PrOH solution of **1**, EtOH solution of **2** and MeOH solution of **3** were respectively sealed in three glass vials under inert atmosphere and stored in 5 °C fridge for about 1–3 days to promote optimal crystal growth.

**Table S1.** Crystal Data and Structure Refinement Parameters for **1–3**

Compound	<b>1</b>	<b>2</b>	<b>3</b>
Shape	Block	Block	Block
Color	Yellow	Yellow	Yellow
Method	Cooling	Cooling	Cooling
Time	1 week	3 days	1 day
Temperature	5 °C	5 °C	5 °C

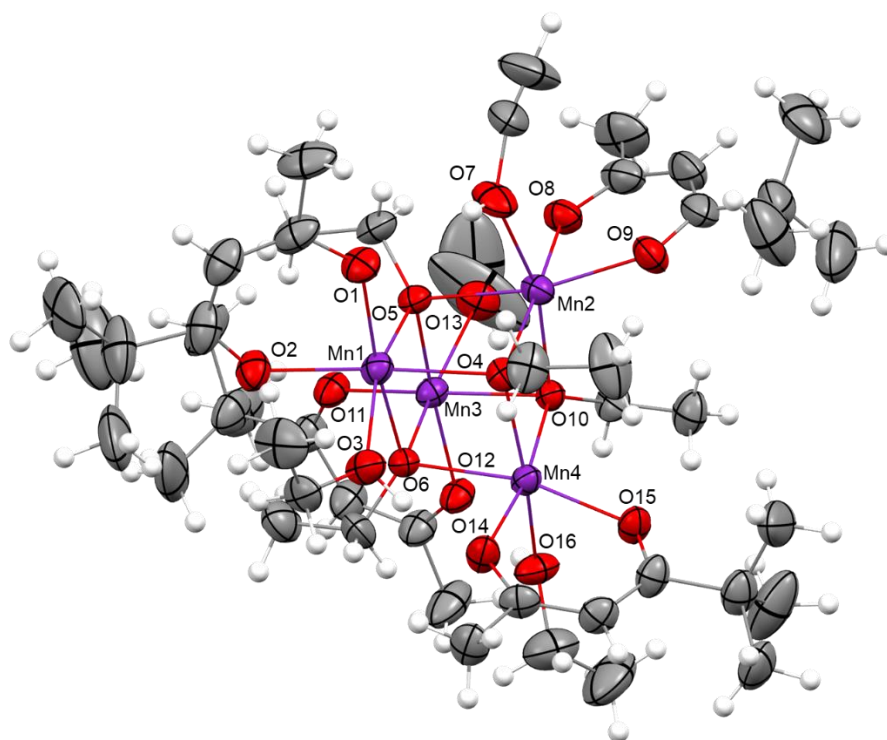
## Solid State Structures of 1–3



**Figure S1.** Solid state structure of **1** drawn with the thermal ellipsoids at the 40% probability level. Hydrogen atoms are represented by spheres of arbitrary radius. Only metal and oxygen atoms are labeled. Mn<sup>II</sup>, purple; O, red; C, grey; H, white.

**Table S2.** Selected bond distances in the structure **1**

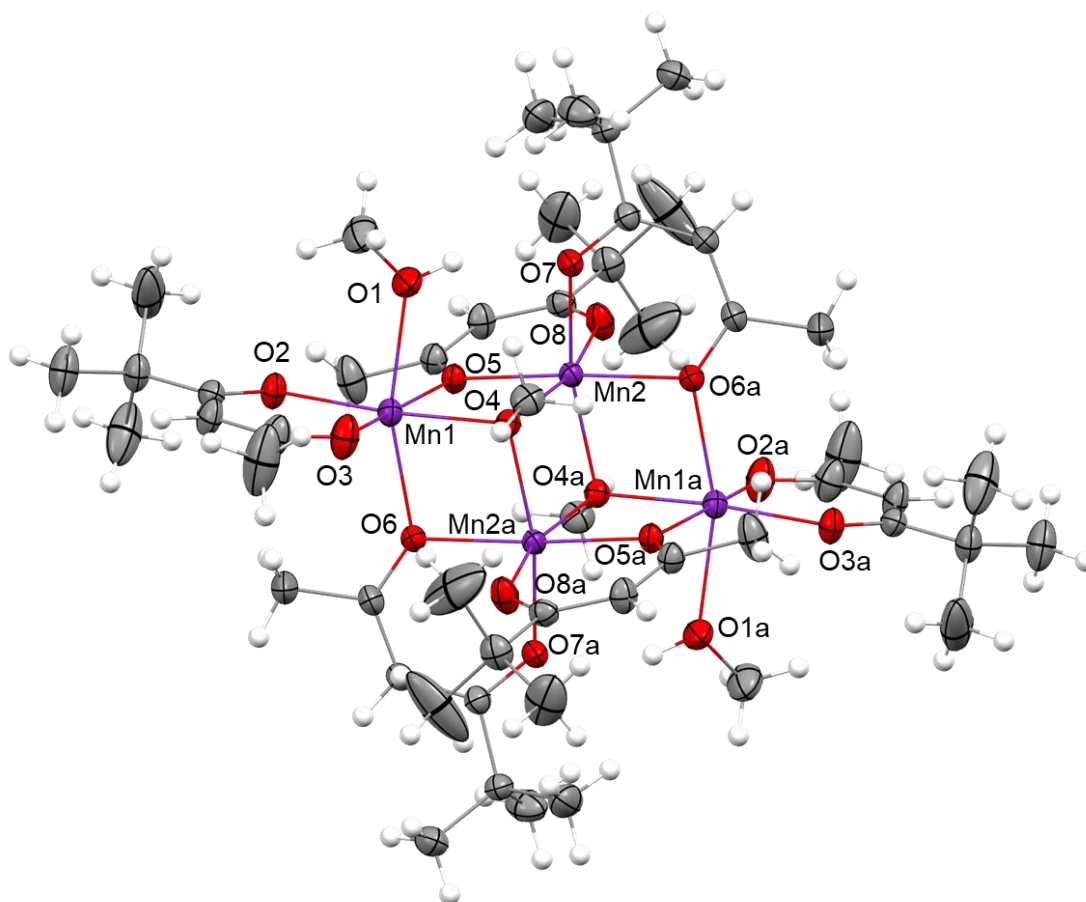
Bond Distances			
Mn1–O1	2.128(3)	Mn2–O5	2.214(2)
Mn1–O2	2.120(2)	Mn2–O6	2.203(2)
Mn1–O3	2.197(2)	Mn2–O7	2.146(2)
Mn1–O4	2.153(2)	Mn2–O8	2.206(2)
Mn1–O5	2.214(2)	Mn2–O9	2.127(3)
Mn1–O6	2.196(3)	Mn2–O10	2.110(2)



**Figure S2.** Solid state structure of **2** drawn with the thermal ellipsoids at the 40% probability level. Hydrogen atoms are represented by spheres of arbitrary radius. Only metal and oxygen atoms are labeled. Mn<sup>II</sup>, purple; O, red; C, grey; H, white.

**Table S3.** Selected bond distances in the structure **2**

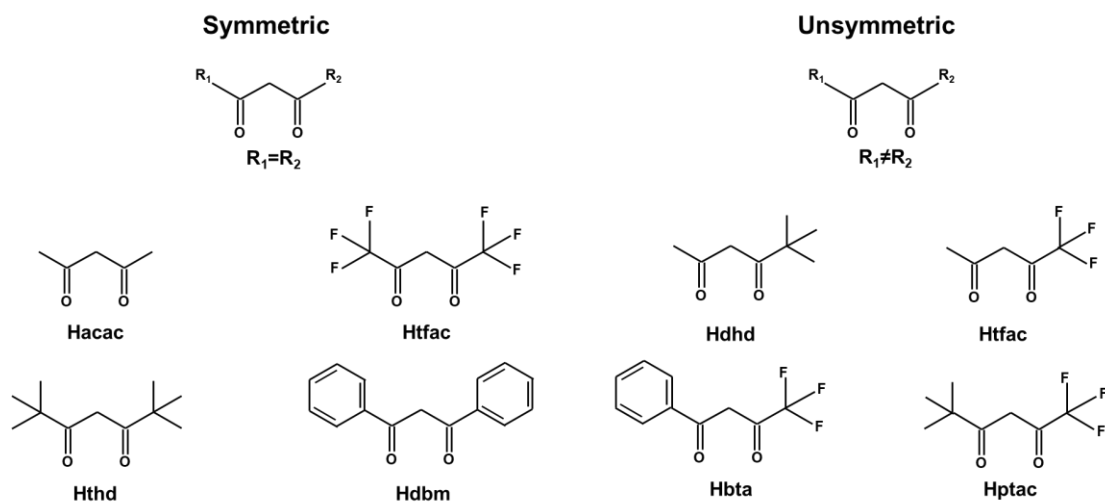
Bond Distances			
Mn1–O1	2.180(3)	Mn3–O5	2.169(3)
Mn1–O2	2.132(6)	Mn3–O6	2.195(4)
Mn1–O3	2.284(9)	Mn3–O10	2.212(4)
Mn1–O4	2.208(4)	Mn3–O11	2.128(5)
Mn1–O5	2.187(4)	Mn3–O12	2.158(3)
Mn1–O6	2.174(3)	Mn3–O13	2.248(7)
Mn2–O4	2.174(4)	Mn4–O4	2.171(3)
Mn2–O5	2.211(4)	Mn4–O6	2.223(4)
Mn2–O7	2.252(4)	Mn4–O10	2.176(4)
Mn2–O8	2.164(4)	Mn4–O14	2.192(4)
Mn2–O9	2.117(5)	Mn4–O15	2.127(5)
Mn2–O10	2.187(4)	Mn4–O16	2.232(4)



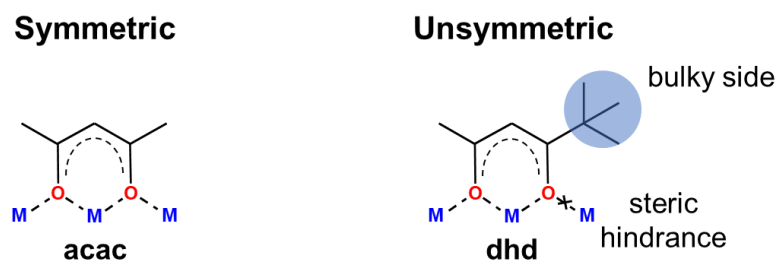
**Figure S3.** Solid state structure of **3** drawn with the thermal ellipsoids at the 40% probability level. Hydrogen atoms are represented by spheres of arbitrary radius. Only metal and oxygen atoms are labeled. Mn<sup>II</sup>, purple; O, red; C, grey; H, white.

**Table S4.** Selected bond distances in the structure **3**

Bond Distances			
Mn1–O1, Mn1a–O1a	2.278(2)	Mn2–O4, Mn2a–O4a	2.151(18)
Mn1–O2, Mn1a–O2a	2.087(19)	Mn2–O5, Mn2a–O5a	2.188(19)
Mn1–O3, Mn1a–O3a	2.116(2)	Mn2–O7, Mn2a–O7a	2.141(18)
Mn1–O4, Mn1a–O4a	2.142(17)	Mn2–O8, Mn2a–O8a	2.080(2)
Mn1–O5, Mn1a–O5a	2.232(19)	Mn2–O4a, Mn2a–O4	2.147(17)
Mn1–O6, Mn1a–O6a	2.266(18)	Mn2–O6a, Mn2a–O6	2.184(19)



**Figure S4.** Symmetric and unsymmetric diketones and their molecular structures.

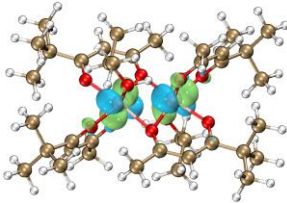
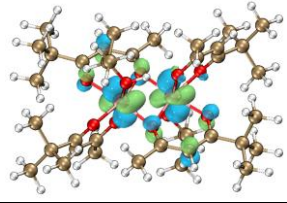
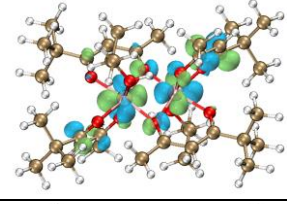
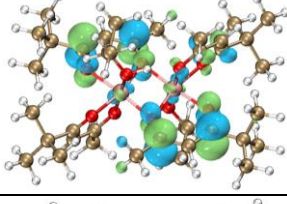
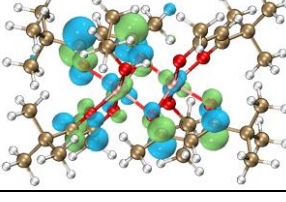


## Theoretical Calculations

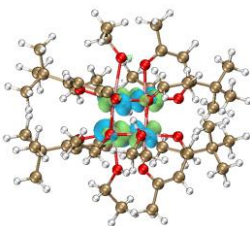
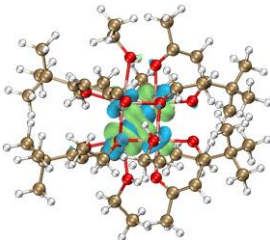
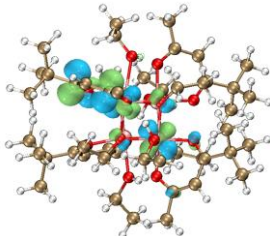
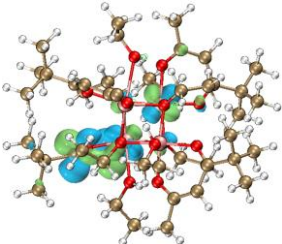
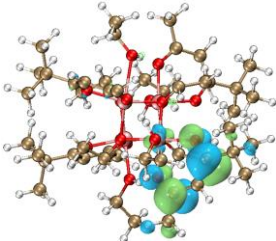
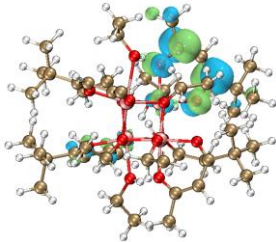
All calculations were performed with ORCA 5.0.4. [1] The geometry optimization of all structures were performed using **unrestricted** PBE hybrid functional under def2-SVP level, and the energy was calculated using the same method under def2-TZVP level. [2, 3] The MO diagrams were generated by Multiwfn 3.8 dev and were plotted by VMD. [4] To compare the stability of different alcohol ligands in the  $Mn_2$  complexes, the coordinated  $iPrOH$  ligand (in **1-*iPr***) was changed to EtOH (**1-Et**) and MeOH (**1-Me**) but the interstitial one was removed. All three structures were optimized, then the alkyl groups were substituted with H atoms and the energy was calculated for stability comparison. Similarly, in the  $Mn_4$  complexes, EtOH/EtO for **2-Et** and MeOH/MeO for **3-Me** were changed (i.e. **2-Me**, **2-*iPr***, **3-Et**, **3-*iPr***) for optimization and energy comparison accordingly.



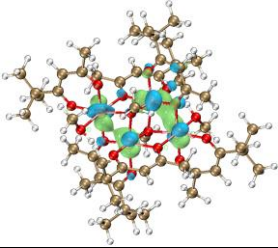
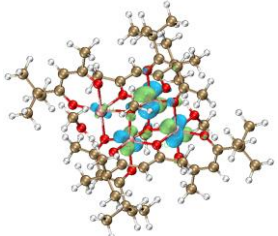
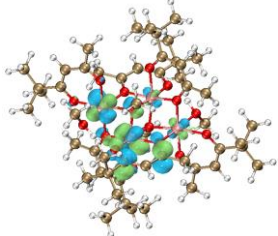
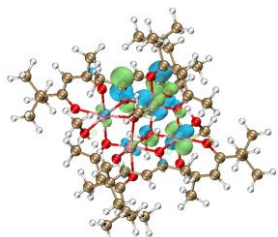
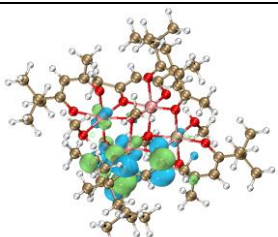
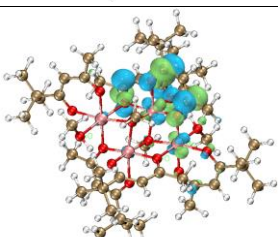
**Table S5.** Orbital composition analysis in **1**.

Orbital	Geometry	Energy	Composition
HOMO-1		-4.41 eV	Mn: 89.3% C,H,O: 20.7%
HOMO		-4.26 eV	Mn: 78.1% C,H,O: 21.9%
LUMO		-1.44 eV	Mn: 62.6% C,H,O: 37.4%
LUMO+1		-0.96 eV	Mn: 4.3% C,H,O: 95.7%
LUMO+2		-0.81 eV	Mn: 10.6% C,H,O: 89.4%

**Table S6.** Orbital composition analysis in **2**.

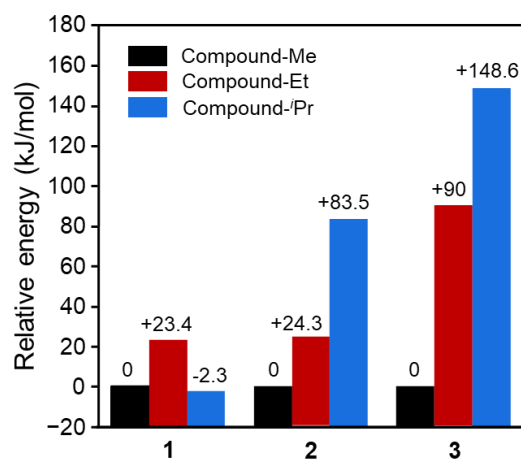
Orbital	Geometry	Energy	Composition
HOMO-1		-3.85 eV	Mn: 88.6% C,H,O: 11.4%
HOMO		-3.67 eV	Mn: 88.2% C,H,O: 11.8%
LUMO		-1.10 eV	Mn: 57.2% C,H,O: 42.8%
LUMO+1		-0.96 eV	Mn: 40.8% C,H,O: 59.2%
LUMO+2		-0.72 eV	Mn: 5.6% C,H,O: 94.4%
LUMO+3		-0.58 eV	Mn: 5.7% C,H,O: 94.3%

**Table S7.** Orbital composition analysis in **3**.

Orbital	Geometry	Energy	Composition
HOMO-1		-4.22 eV	Mn: 85.8% C,H,O: 14.2%
HOMO		-4.08 eV	Mn: 85.8% C,H,O: 14.2%
LUMO		-1.30 eV	Mn: 68.9% C,H,O: 31.1%
LUMO+1		-1.12 eV	Mn: 51.1% C,H,O: 48.9%
LUMO+2		-0.71 eV	Mn: 18.6% C,H,O: 81.4%
LUMO+3		-0.62 eV	Mn: 16.3% C,H,O: 83.7%

**Table S8.** Energy comparison of **1–3** with different alcoho/alkoxide ligands.

Complex	Energy (Hartree)	Relative Energy to <b>1-Me/2-Me/3-Me</b> (kJ/mol)
<b>1-Me</b>	-4305.686632439016	0
<b>1-Et</b>	-4305.677723127723	+23.4
<b>1-iPr</b>	-4305.687509771328	-2.3
<b>2-Me</b>	-7063.264764274314	0
<b>2-Et</b>	-7063.255518494434	+24.3
<b>2-iPr</b>	-7063.223714198468	+83.5
<b>3-Me</b>	-7684.554415351536	0
<b>3-Et</b>	-7684.519785911066	+90.0
<b>3-iPr</b>	-7684.497806268972	+148.6



**Figure S6.** Theoretical calculations for relative energies of rhombic, cubic and defective-dicubic structures with different alcohol/alkoxide ligands.

**Table S9.** Cartesian coordinates of the H-substituted **1-Me**.

Total Energy: -4305.686632439016 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	9.255767	10.396284	5.948604	C	15.321211	7.500489	2.181890
Mn	10.540793	8.843717	4.428393	H	15.940580	8.186299	2.780096
O	10.682186	10.774142	4.703654	H	15.819368	7.364638	1.209499
O	8.973094	8.499066	5.518571	H	15.306478	6.521113	2.683184
O	11.999978	8.822903	3.109197	C	14.001306	9.377057	1.202388
O	7.849369	10.423988	7.314641	H	12.998815	9.782316	1.012233
O	7.990304	10.872691	4.506616	H	14.505951	9.225939	0.235409
O	11.807419	8.399547	5.890900	H	14.574994	10.126174	1.770435
O	10.535227	6.929943	4.013758	C	7.961002	14.816780	6.111040
O	9.334707	9.393235	2.868531	H	7.740919	14.835643	5.031889
H	8.647530	9.992777	3.248977	H	7.602736	15.761443	6.550324
O	9.332298	12.295178	6.427672	H	7.399604	13.981892	6.553268
O	10.450010	9.819991	7.504089	C	13.099027	7.045507	1.137305
H	11.129739	9.212414	7.118986	H	13.030429	6.074796	1.651258
C	8.524325	7.400432	6.009550	H	13.575417	6.881766	0.157690
C	13.660399	7.878262	4.506484	H	12.078368	7.419934	0.977009
H	14.665652	7.466584	4.531078	C	9.742496	14.652619	7.868712
C	6.720627	10.965541	7.175029	H	9.202911	13.833492	8.361577
C	9.847503	13.265908	5.815825	H	9.418171	15.606744	8.312723
C	13.126123	8.280323	3.264749	H	10.817516	14.528566	8.074652
C	6.794113	11.253884	4.693128	C	4.561442	11.784724	8.300608
C	10.714582	13.119016	4.713235	H	4.582045	12.760670	7.792606
H	11.145004	14.000135	4.245268	H	4.086927	11.934682	9.282681
C	13.000796	7.996008	5.737185	H	3.917867	11.105816	7.720389
C	11.112090	11.877884	4.216408	C	5.873137	9.889504	9.257774
C	8.956059	6.150034	5.570561	H	5.274716	9.147859	8.705835
H	8.489383	5.279216	6.022871	H	5.394915	10.050370	10.236580
C	13.913593	8.050568	1.963547	H	6.874332	9.470242	9.424764
C	12.101917	11.783126	3.105236	C	6.809687	12.206383	9.301240
H	13.025503	11.311104	3.473014	H	7.828220	11.817950	9.439492
H	12.337677	12.770592	2.690739	H	6.881108	13.176816	8.787549
H	11.706498	11.115631	2.328151	C	10.227132	15.795001	5.700409
C	6.158293	11.350793	5.939359	H	11.314340	15.699742	5.844066
H	5.151469	11.759654	5.936010	H	9.913643	16.751366	6.147100
C	7.473453	7.512697	7.061611	H	10.025391	15.855257	4.620323
H	7.866242	8.101864	7.901404	C	10.365406	4.582204	4.093971
H	7.141165	6.526214	7.406256	C	10.190339	4.546198	2.570987
H	6.614427	8.076901	6.668166	H	9.130960	4.663401	2.292358
C	6.039749	11.639719	3.449366	H	10.544688	3.584770	2.167020
H	6.630671	12.373550	2.879915	H	10.760014	5.357404	2.098962
H	5.048604	12.056622	3.665933	C	9.564312	3.447574	4.726409

H	6.356322	12.375587	10.290797	H	9.686324	3.419069	5.819775
H	5.914909	10.755018	2.804264	H	9.914958	2.482065	4.329766
C	9.940983	5.975271	4.574250	H	8.490196	3.530541	4.500517
C	13.727118	7.624288	7.001375	C	11.850667	4.424946	4.448345
H	13.877479	8.524522	7.618997	H	12.438344	5.252631	4.026960
H	14.705256	7.167289	6.808035	H	12.240193	3.471715	4.056850
H	13.105953	6.930079	7.587707	H	11.996163	4.430592	5.540330
C	5.964335	11.213366	8.491704	H	8.907726	8.592663	2.465020
C	9.466597	14.648026	6.360872	H	9.914113	9.345293	8.192221

**Table S10.** Cartesian coordinates of the H-substituted **1-Et.**

Total Energy: -4305.677723127723 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	9.176645	10.393206	5.989215	H	16.086741	8.015173	2.991517
Mn	10.545620	8.793947	4.384189	H	15.999635	7.237606	1.397373
O	10.583305	10.789438	4.695619	H	15.389331	6.380647	2.825937
O	8.876011	8.492346	5.468647	C	14.264481	9.333365	1.382181
O	12.149023	8.782408	3.147278	H	13.286691	9.787400	1.173994
O	7.771101	10.409195	7.346972	H	14.801365	9.200263	0.429938
O	7.932704	10.926871	4.556338	H	14.845091	10.033624	2.003863
O	11.855072	8.341677	5.969661	C	8.558217	14.521843	7.657730
O	10.512269	6.831700	4.001594	H	7.646853	13.934299	7.481006
O	9.172834	9.574923	2.632414	H	8.272281	15.521495	8.019579
H	8.574514	10.138994	3.176624	H	9.127312	14.014196	8.449542
O	9.305076	12.272065	6.509383	C	13.275591	7.038503	1.194417
O	10.380528	9.757407	7.516717	H	13.147746	6.055078	1.672972
H	11.048395	9.140353	7.120484	H	13.786432	6.886886	0.230331
C	8.414352	7.388855	5.942240	H	12.277241	7.457766	1.007378
C	13.728438	7.789682	4.616393	C	10.659224	15.443340	6.662226
H	14.726507	7.362965	4.669620	H	11.286939	14.926127	7.404121
C	6.676908	11.022395	7.231064	H	10.404211	16.435887	7.066397
C	9.737024	13.251264	5.851743	H	11.263315	15.594399	5.755906
C	13.251961	8.211358	3.354621	C	4.887296	12.356289	8.481089
C	6.765066	11.383367	4.758262	H	5.385654	13.299363	8.210146
C	10.516515	13.129040	4.679442	H	4.424773	12.491528	9.471142
H	10.862924	14.030145	4.175887	H	4.070810	12.181467	7.764938
C	13.047736	7.927810	5.833152	C	5.108219	9.884331	8.773750
C	10.931150	11.904576	4.165727	H	4.418784	9.668564	7.942461
C	8.845121	6.132126	5.517059	H	4.514532	9.957626	9.698968
H	8.353479	5.273731	5.967228	H	5.798032	9.035049	8.878375
C	14.092483	7.983545	2.087453	C	6.863184	11.422219	9.683759
C	11.822271	11.821192	2.972190	H	7.593443	10.604645	9.737721
H	12.775671	11.350496	3.252723	H	6.321792	11.484188	10.640449
H	12.011883	12.808916	2.535123	H	7.420927	12.359889	9.540896
H	11.355053	11.151251	2.235356	C	8.540319	15.363356	5.308926
C	6.146542	11.497064	6.010736	H	9.098151	15.501097	4.371196
H	5.167944	11.970679	6.027416	H	8.236928	16.358264	5.672343
C	7.338451	7.504488	6.970096	H	7.627832	14.790541	5.080797
H	7.712522	8.095800	7.818151	C	10.286728	4.496069	4.147863
H	6.993323	6.520553	7.309353	C	10.171347	4.416150	2.620546
H	6.491054	8.069256	6.552272	H	9.123803	4.529088	2.298523
C	6.036574	11.845678	3.525875	H	10.535817	3.441802	2.258843
H	6.657242	12.586074	2.997544	H	10.761979	5.213255	2.149156
H	5.056044	12.283508	3.749768	C	9.445883	3.392250	4.782808



H	5.895385	10.995083	2.839715	H	9.527331	3.394360	5.880353
C	9.867868	5.911189	4.564895	H	9.796346	2.410615	4.427786
C	13.759291	7.574275	7.111576	H	8.382113	3.482866	4.514681
H	13.939256	8.493199	7.692840	C	11.755143	4.331804	4.565438
H	14.722558	7.079462	6.937358	H	12.370245	5.136706	4.138723
H	13.114681	6.923905	7.721802	H	12.144564	3.360350	4.221857
C	5.877182	11.191654	8.534673	H	11.858479	4.373002	5.661501
C	9.379670	14.647727	6.376765	H	8.686583	8.838647	2.176885
C	15.465439	7.370482	2.351051	H	9.840798	9.282134	8.201447

**Table S11.** Cartesian coordinates of the H-substituted **1-iPr**.

Total Energy: -4305.687509771328 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	9.180858	10.422729	6.044388	H	15.824691	8.196967	2.825903
Mn	10.426435	8.838732	4.496464	H	15.705524	7.351884	1.268833
O	10.583540	10.766745	4.754218	H	15.210232	6.523569	2.757026
O	8.864202	8.526141	5.601632	C	13.862190	9.335070	1.231472
O	11.878764	8.797223	3.164889	H	12.853865	9.726483	1.041782
O	7.801418	10.446932	7.437776	H	14.359640	9.167774	0.263154
O	7.892637	10.892239	4.628171	H	14.435368	10.100718	1.777651
O	11.706220	8.413304	5.947265	C	8.491834	14.641328	7.508678
O	10.411361	6.923720	4.102304	H	7.571736	14.190453	7.109950
O	9.125482	9.343861	2.971949	H	8.265310	15.659070	7.862134
H	8.558351	10.026828	3.411993	H	8.805775	14.034753	8.368537
O	9.277849	12.324295	6.506867	C	12.986575	6.992354	1.222128
O	10.470007	9.911463	7.567774	H	12.935144	6.031618	1.756562
H	11.046742	9.229493	7.134681	H	13.459014	6.815777	0.242885
C	8.329479	7.433892	6.016615	H	11.959910	7.350551	1.063336
C	13.561088	7.898821	4.568243	C	10.871655	15.252353	7.053979
H	14.573578	7.505040	4.594215	H	11.226889	14.613156	7.877337
C	6.655620	10.954251	7.315617	H	10.688750	16.259151	7.462389
C	9.858093	13.272098	5.924510	H	11.680362	15.328730	6.312182
C	13.010941	8.270157	3.322125	C	4.489859	11.727601	8.463281
C	6.690453	11.251419	4.831457	H	4.522368	12.721728	7.991756
C	10.765801	13.098901	4.854729	H	4.014128	11.843857	9.449373
H	11.254844	13.973582	4.429322	H	3.840851	11.077537	7.856533
C	12.909008	8.031498	5.798735	C	5.774057	9.770317	9.325213
C	11.107207	11.858779	4.329409	H	5.185531	9.061335	8.722203
C	8.717854	6.179334	5.552296	H	5.275713	9.879999	10.301312
H	8.191664	5.319256	5.957267	H	6.771479	9.341517	9.493952
C	13.794469	8.024052	2.021259	C	6.723495	12.067294	9.525597
C	12.129767	11.742368	3.249463	H	7.749276	11.684545	9.620702
H	13.015874	11.213836	3.634140	H	6.275465	12.137254	10.529477
H	12.429797	12.728420	2.873844	H	6.773359	13.079925	9.100610
H	11.731846	11.121208	2.436130	C	9.116503	15.579950	5.283481
C	6.071985	11.336049	6.086000	H	9.884730	15.687692	4.504319
H	5.055073	11.719588	6.095695	H	8.876653	16.587328	5.658538
C	7.234821	7.562704	7.020127	H	8.211083	15.169164	4.811018
H	7.612536	8.097513	7.901354	C	10.177559	4.582302	4.157081
H	6.834385	6.584137	7.310195	C	10.068472	4.548682	2.627851
H	6.426113	8.185840	6.607736	H	9.023088	4.677437	2.304287
C	5.914168	11.614396	3.594788	H	10.429138	3.583715	2.238281
H	6.468750	12.380058	3.030256	H	10.667505	5.354125	2.182817
H	4.905171	11.982785	3.817082	C	9.330826	3.462263	4.754797

H	5.832089	10.729887	2.942280	H	9.404140	3.434153	5.852432
C	9.757198	5.983498	4.617376	H	9.682356	2.490603	4.374813
C	13.644709	7.708943	7.069698	H	8.269185	3.561622	4.481555
H	13.740590	8.622168	7.679736	C	11.643403	4.400236	4.576134
H	14.646705	7.301497	6.887437	H	12.263347	5.216324	4.178707
H	13.056371	6.988219	7.658420	H	12.032491	3.438958	4.204622
C	5.886834	11.136382	8.638361	H	11.740707	4.405943	5.673420
C	9.581455	14.689641	6.442276	H	8.588932	8.561232	2.679281
C	15.210198	7.495402	2.241507	H	9.979158	9.528909	8.341576

**Table S12.** Cartesian coordinates of the H-substituted **2-Me**.

Total Energy: -7063.264764274314 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	11.297806	4.366281	10.347066	H	4.344920	3.333553	13.646724
Mn	10.472476	6.189712	11.895878	C	13.297015	5.579611	15.083486
Mn	9.933455	6.862475	9.016997	H	14.068238	6.244355	14.664526
Mn	8.269227	5.066997	9.854587	H	13.612135	4.546505	14.862961
O	9.977530	4.898111	8.827037	H	13.257625	5.706756	16.172467
O	9.715265	4.442391	11.499592	C	13.530243	6.919554	6.041249
O	11.499884	6.316963	10.234256	H	14.217546	7.396039	6.757692
O	8.888844	6.770094	10.667878	H	14.111421	6.632045	5.150882
O	10.806830	2.471714	10.045332	H	13.128191	6.013805	6.512760
O	6.962046	5.395666	8.255638	C	3.006580	4.254347	11.441228
O	6.610522	4.940806	11.054485	H	2.382706	4.070993	12.329815
O	11.989558	5.820906	13.142204	H	2.980139	3.344719	10.821551
O	12.866106	4.125435	9.179150	H	2.535714	5.072627	10.876076
O	8.315156	7.515337	7.861708	C	8.690013	6.544210	17.086590
H	7.695846	6.742869	7.909341	H	9.112551	5.576262	17.396493
O	11.064843	7.059335	7.441000	H	7.777282	6.711696	17.679291
O	9.280877	6.353330	13.452497	H	9.407599	7.335484	17.352392
O	12.724708	3.832701	11.785691	C	10.961646	11.002725	9.372501
H	12.637407	4.592681	12.417421	H	9.957330	11.326607	9.685341
O	10.288033	8.751234	9.474390	H	11.387409	11.744935	8.685842
O	10.798070	8.222704	12.077428	H	11.587108	10.968457	10.280120
H	10.670787	8.583688	11.167481	C	7.744316	7.925489	15.229818
O	8.101313	2.735069	9.644203	H	8.452237	8.741621	15.445483
H	9.056131	2.510671	9.745803	H	6.825045	8.108534	15.808186
C	11.524327	1.569826	9.495365	H	7.503100	7.960453	14.158937
C	5.692055	5.249894	8.270497	C	15.164455	4.327458	7.652079
C	10.871566	0.222700	9.349163	H	16.240902	4.472737	7.471631
H	11.581936	-0.557463	9.047672	H	14.754663	5.242169	8.096669
H	10.078356	0.277720	8.584820	H	14.673185	4.172328	6.679647
H	10.390408	-0.063776	10.296770	C	4.427484	4.600771	11.881709
C	12.827129	1.767463	9.039358	C	15.658986	3.391252	9.914924
H	13.365065	0.892872	8.681987	H	15.525653	2.544032	10.605521
C	13.448671	3.037953	8.939724	H	15.253965	4.289039	10.402938
C	5.408351	4.820008	10.717641	H	16.739002	3.530151	9.745188
C	4.923263	4.921157	9.387250	C	7.338044	5.452369	15.286232
H	3.854974	4.807408	9.221983	H	7.116735	5.438023	14.210918
C	11.977239	5.861529	14.419217	H	6.400293	5.612262	15.841068
C	9.553696	6.339714	14.676841	H	7.737497	4.464759	15.566438
C	14.939156	3.136396	8.579919	C	12.958081	9.146073	5.055114
C	11.576272	8.096878	6.944531	H	12.165634	9.859631	4.781603
C	5.010653	5.480797	6.949074	H	13.517488	8.903343	4.138383

H	5.516423	4.893408	6.167766	H	13.654095	9.649810	5.742611
H	5.111441	6.542390	6.669135	C	4.403892	5.910193	12.683666
H	3.943778	5.225811	6.970009	H	3.763209	5.801880	13.573174
C	10.878234	9.630729	8.762983	H	4.008333	6.738399	12.074901
C	10.852303	6.130046	15.201673	H	5.415495	6.181171	13.014650
H	10.990000	6.138638	16.280145	C	11.478018	7.177831	4.638710
C	8.347067	6.563719	15.600006	H	11.039062	6.265726	5.066933
C	11.467653	9.383972	7.520986	H	12.054120	6.901938	3.741769
H	11.943060	10.224729	7.022271	H	10.658220	7.841335	4.321676
C	15.502661	1.873937	7.930152	H	7.745371	2.463903	8.757737
H	14.962559	1.617546	7.005553	H	10.007578	4.462043	7.935414
H	15.463654	1.006262	8.605193	H	8.591877	7.697086	6.925524
H	16.559922	2.034547	7.667324	H	11.720821	8.401229	12.397912
C	12.388287	7.866971	5.661837	H	13.636821	3.782531	11.396357
C	4.974416	3.464240	12.752837	H	9.503456	3.762751	12.191889
H	6.002281	3.678972	13.071392	H	8.255619	7.488506	10.930479
H	4.984438	2.513114	12.197815	H	12.388056	6.758789	10.189656

**Table S13.** Cartesian coordinates of the H-substituted **2-Et.**

Total Energy: -7063.255518494434 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	11.271454	4.260877	10.242776	H	4.687003	3.770505	13.816550
Mn	10.464864	6.057342	11.947422	C	13.106397	5.284791	15.318107
Mn	10.047303	6.822713	8.941588	H	13.982757	5.788542	14.881751
Mn	8.404731	5.027105	9.715774	H	13.258258	4.201291	15.185308
O	10.057931	4.889433	8.658029	H	13.057934	5.502593	16.392201
O	9.590384	4.348898	11.293158	C	13.495409	7.167285	5.552758
O	11.573383	6.196661	10.292301	H	14.208680	7.713982	6.188171
O	8.874819	6.773209	10.531515	H	13.969320	6.992146	4.573886
O	10.822652	2.392247	9.813477	H	13.299938	6.193256	6.019805
O	7.134991	5.420331	8.216580	C	3.924999	2.893938	11.328632
O	6.824622	4.668401	10.879973	H	3.236726	2.596611	12.135758
O	11.902028	5.551363	13.315274	H	4.652742	2.079204	11.189386
O	12.963680	4.035852	9.272128	H	3.338393	2.987099	10.403052
O	8.432670	7.530081	7.837110	C	8.957895	8.293615	16.531495
H	7.799055	6.767812	7.827979	H	9.780081	7.985024	17.192862
O	11.126211	7.064021	7.301721	H	8.144658	8.677985	17.167215
O	9.269650	6.569705	13.505932	H	9.321585	9.124920	15.908518
O	12.499985	3.599459	11.822084	C	11.264733	10.910210	9.381367
H	12.479422	4.351271	12.470077	H	10.311337	11.265395	9.801967
O	10.466327	8.699233	9.405231	H	11.672713	11.672336	8.705854
O	11.048579	8.422754	12.018429	H	11.962823	10.775663	10.223888
H	10.740841	8.614796	11.100842	C	7.248518	7.618953	14.842234
O	8.273659	2.978335	9.221403	H	7.530505	8.442855	14.171180
H	9.160153	2.592343	9.421525	H	6.447688	7.972019	15.509832
C	11.627222	1.479817	9.417004	H	6.851162	6.812882	14.212050
C	5.873305	5.229668	8.188159	C	15.086599	3.814601	7.303509
C	11.018347	0.119012	9.232400	H	16.126928	3.977610	6.980542
H	11.769132	-0.654075	9.027310	H	14.585757	4.789811	7.359884
H	10.309891	0.148677	8.388715	H	14.577321	3.213244	6.534490
H	10.441704	-0.157320	10.128899	C	4.630737	4.205897	11.697513
C	12.978692	1.681722	9.150165	C	15.745526	3.988866	9.717078
H	13.566050	0.807586	8.882019	H	15.747255	3.499891	10.703156
C	13.582614	2.963730	9.075336	H	15.226272	4.949560	9.817945
C	5.612082	4.585841	10.576266	H	16.790295	4.180522	9.426168
C	5.100661	4.817905	9.274927	C	7.997779	5.971957	16.562522
H	4.030278	4.699539	9.110820	H	7.631999	5.128588	15.957331
C	11.867872	5.714898	14.581318	H	7.180108	6.295068	17.226533
C	9.548000	6.633284	14.728232	H	8.821697	5.603509	17.191015
C	15.055927	3.110985	8.665772	C	12.490923	9.283515	4.688485
C	11.558278	8.117824	6.770765	H	11.588407	9.906506	4.592044
C	5.210349	5.500209	6.865210	H	12.876896	9.094380	3.674732

H	5.757429	4.972525	6.069221	H	13.255379	9.864351	5.225962
H	5.266290	6.576541	6.634227	C	3.593768	5.323880	11.869995
H	4.156019	5.196571	6.849847	H	2.903285	5.070585	12.690225
C	11.056278	9.584852	8.703637	H	2.995770	5.475414	10.959716
C	10.788458	6.240304	15.292871	H	4.079856	6.279562	12.117113
H	10.908085	6.328193	16.372035	C	11.220802	7.144781	4.508688
C	8.439960	7.138292	15.666985	H	10.952430	6.203087	5.004720
C	11.531797	9.384017	7.405312	H	11.682937	6.913655	3.536239
H	11.979420	10.237258	6.902475	H	10.294459	7.708561	4.317228
C	15.796909	1.779278	8.564280	H	9.302788	3.623759	11.907577
H	15.386443	1.135388	7.771916	H	13.425611	3.432268	11.503787
H	15.766685	1.222521	9.513474	H	8.059386	2.869021	8.257979
H	16.854629	1.964926	8.321298	H	8.211444	7.478039	10.753320
C	12.189783	7.953814	5.377657	H	10.089555	4.475606	7.755922
C	5.391193	4.017290	13.007203	H	8.712564	7.768198	6.914608
H	5.937209	4.929338	13.285019	H	12.021658	8.578066	12.141087
H	6.130753	3.208878	12.928797	H	12.482997	6.594969	10.291333

**Table S14.** Cartesian coordinates of the H-substituted **2-iPr**.

Total Energy: -7063.223714198468 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	11.334837	4.174038	10.396422	H	4.543428	2.463735	13.394066
Mn	10.351164	6.111379	12.007675	C	12.891782	5.566086	15.477540
Mn	10.035453	6.822763	8.915303	H	13.798069	5.864342	14.930301
Mn	8.281995	4.914050	9.738780	H	12.929603	4.472064	15.607303
O	9.954158	4.838402	8.604702	H	12.896925	6.027115	16.473016
O	9.621288	4.291266	11.518959	C	13.804029	7.354764	5.765463
O	11.646123	6.159180	10.472724	H	14.393644	7.965204	6.466064
O	8.788927	6.695224	10.521155	H	14.388039	7.230066	4.839769
O	10.953735	2.244733	9.903472	H	13.657139	6.365102	6.216692
O	6.952366	5.558785	8.373151	C	3.335626	3.077599	11.027811
O	6.721189	4.348264	10.907208	H	2.729244	2.577305	11.799101
O	11.696656	5.637018	13.444086	H	3.677607	2.310571	10.315549
O	13.094159	3.895180	9.390918	H	2.669781	3.766271	10.489015
O	8.507378	7.350326	7.424741	C	8.681005	8.606791	16.433570
H	7.765403	6.714270	7.579476	H	9.604668	8.468362	17.013506
O	11.274070	7.094269	7.298138	H	7.894418	8.939083	17.129535
O	9.064238	6.697283	13.548630	H	8.852179	9.418402	15.710403
O	12.604720	3.673027	12.094614	C	11.073840	11.009590	9.267106
H	12.442643	4.338661	12.808717	H	10.064673	11.300652	9.597141
O	10.504257	8.729297	9.398404	H	11.457638	11.762460	8.567931
O	10.713867	8.367016	12.130541	H	11.717025	11.000803	10.161007
H	10.642060	8.697346	11.207312	C	6.942930	7.587860	14.971241
O	8.150455	2.766603	9.159723	H	7.075788	8.363105	14.205898
H	9.007423	2.409939	9.460435	H	6.164925	7.923185	15.674093
C	11.753662	1.347656	9.483083	H	6.585267	6.683973	14.462096
C	5.678618	5.541426	8.450498	C	15.066022	3.863454	7.268292
C	11.194909	-0.043944	9.362967	H	16.082139	4.029631	6.876845
H	11.974624	-0.785075	9.147908	H	14.614540	4.839047	7.484626
H	10.452701	-0.074491	8.551386	H	14.469962	3.374941	6.482341
H	10.674197	-0.323647	10.291130	C	4.518873	3.792963	11.689157
C	13.082435	1.560964	9.107406	C	15.920392	3.740855	9.619599
H	13.651318	0.694153	8.783321	H	16.029965	3.116985	10.520204
C	13.680627	2.839859	9.052537	H	15.416129	4.673425	9.905790
C	5.492700	4.368067	10.642976	H	16.929591	3.983478	9.251327
C	4.941368	4.960389	9.481766	C	7.979878	6.218796	16.766912
H	3.858935	4.983120	9.379683	H	7.690881	5.275188	16.279600
C	11.669135	5.937985	14.683057	H	7.157521	6.521974	17.434543
C	9.340910	6.837813	14.762987	H	8.864804	6.020798	17.388211
C	15.121585	3.005827	8.536969	C	12.690079	9.342787	4.741375
C	11.698110	8.157777	6.785995	H	11.747307	9.882314	4.561135
C	4.946819	6.184518	7.305504	H	13.163412	9.159872	3.764346



H	5.232287	5.692385	6.362578	H	13.361585	10.002196	5.311166
H	5.241568	7.242498	7.222811	C	4.005863	4.974452	12.527771
H	3.857532	6.130969	7.420625	H	3.289032	4.616481	13.284153
C	11.026535	9.631664	8.666181	H	3.499971	5.724389	11.901288
C	10.601131	6.542187	15.341873	H	4.834807	5.474447	13.049154
H	10.726983	6.726094	16.407614	C	11.653541	7.085370	4.528942
C	8.237065	7.319478	15.725953	H	11.408621	6.146298	5.041984
C	11.558630	9.429988	7.390162	H	12.240935	6.850373	3.627797
H	11.961876	10.301660	6.882011	H	10.713980	7.557088	4.203683
C	15.813009	1.681860	8.218380	H	8.045983	2.666527	8.177318
H	15.305843	1.137589	7.407588	H	8.111956	7.394615	10.717651
H	15.864221	1.023700	9.099227	H	11.618260	8.553197	12.495861
H	16.845550	1.876674	7.889303	H	12.548915	6.568365	10.532579
C	12.453313	8.010475	5.450941	H	13.558740	3.699693	11.820417
C	5.234051	2.806559	12.608246	H	8.867750	7.248384	6.505073
H	6.107271	3.264571	13.084445	H	9.358070	3.608267	12.189986
H	5.580013	1.919241	12.056771	H	9.987209	4.422617	7.703547

**Table S15.** Cartesian coordinates of the H-substituted **3-Me**.

Total Energy: -7684.554415351536 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	5.535479	8.241419	6.591063	O	5.082917	6.374677	6.787024
Mn	2.363367	8.364857	7.185067	O	5.435022	6.372182	9.338260
O	4.170865	8.395955	8.093551	O	2.285017	6.328842	7.049040
O	3.905662	8.402338	5.464941	O	2.648507	6.648961	9.950323
O	6.969312	8.401279	7.860846	O	3.638170	4.596064	8.620696
O	6.656092	8.135867	4.942942	O	8.501230	6.191085	8.748695
O	5.632077	10.161997	6.296295	O	6.719441	4.478328	7.573733
O	0.664270	8.611499	6.127492	O	8.137238	6.489806	6.125261
O	2.422046	10.335874	7.397383	H	7.728880	7.144848	5.502432
O	0.916869	8.212961	8.912125	C	3.024471	6.249149	11.092562
H	1.441405	7.609062	9.495137	C	2.751571	3.776083	8.294608
C	6.331735	8.566675	3.795629	C	1.930321	6.171674	12.165789
C	6.488709	10.989382	6.678387	C	4.355035	5.941588	11.411937
C	7.470362	8.642933	2.769959	H	4.563836	5.618929	12.428410
C	5.020753	8.912507	3.436821	C	8.772520	3.857282	8.572645
H	4.846251	9.276209	2.427471	H	9.412096	3.006734	8.791614
C	0.381726	10.944690	6.354473	C	9.197020	5.150066	8.921521
H	-0.256836	11.794638	6.129099	C	2.882533	2.355762	8.860181
C	-0.020522	9.659821	5.950832	C	1.507076	5.329323	6.823406
C	6.343643	12.424320	6.155970	C	5.474337	6.036385	10.568857
C	7.713960	9.411196	8.144049	C	1.686417	4.083795	7.411877
C	3.886280	8.800658	4.258948	H	0.975136	3.301982	7.150840
C	7.530772	10.670388	7.583522	C	10.592848	5.375380	9.528087
H	8.217543	11.456656	7.893182	C	2.259522	5.161687	13.266896
C	-1.383193	9.444090	5.272123	H	3.125928	5.464976	13.872211
C	7.205323	9.680039	1.676982	H	1.401720	5.072156	13.950946
H	6.352311	9.408076	1.038602	H	2.465358	4.164715	12.847995
H	8.087639	9.759327	1.023311	C	1.795938	7.572485	12.781339
H	7.009894	10.674782	2.106287	H	1.552622	8.322848	12.015419
C	7.603267	7.251998	2.131850	H	0.992755	7.583519	13.535276
H	7.802297	6.482385	2.891738	H	2.732524	7.879711	13.270828
H	8.435236	7.240828	1.409564	C	7.550174	3.598749	7.923481
H	6.681401	6.972320	1.599655	C	0.609933	5.759496	11.505189
C	1.582112	11.206768	7.043767	H	0.699996	4.774052	11.023608
C	8.769058	9.012195	3.495716	H	-0.185493	5.701319	12.263576
H	8.676587	9.985137	4.002383	H	0.292831	6.468540	10.730215
H	9.598030	9.074899	2.774227	C	11.342384	4.078277	9.828880
H	9.035791	8.273531	4.262740	H	11.521105	3.486817	8.918691
C	-2.107369	10.744159	4.927193	H	12.324397	4.313014	10.267865
H	-2.342231	11.334565	5.825247	H	10.796920	3.449229	10.548592
H	-3.060512	10.514211	4.426307	C	0.409113	5.559318	5.839435

H	-1.514826	11.372940	4.245323	H	0.851116	5.734670	4.844934
C	8.775291	9.189089	9.168995	H	-0.275356	4.704696	5.781877
H	8.298381	8.994389	10.143766	H	-0.126579	6.480619	6.101920
H	9.438069	10.057285	9.263947	C	1.557908	1.894528	9.476431
H	9.339643	8.283611	8.917151	H	0.746627	1.839650	8.736433
C	7.660303	12.895547	5.529234	H	1.677906	0.890906	9.914462
H	8.484723	12.915875	6.257209	H	1.235659	2.576068	10.278783
H	7.542754	13.914547	5.127032	C	6.814319	5.715212	11.145750
H	7.960939	12.237574	4.698494	H	7.525283	6.512582	10.895409
C	2.548883	9.180878	3.707105	H	6.769529	5.568850	12.231277
H	1.825512	8.380918	3.914032	H	7.204256	4.798991	10.673114
H	2.582987	9.397378	2.632692	C	7.186651	2.174650	7.595886
H	2.181906	10.069124	4.246779	H	6.755940	2.131320	6.585188
C	1.920937	12.629572	7.402930	H	8.047697	1.497145	7.661670
H	2.267688	12.669195	8.446023	H	6.412678	1.820537	8.293984
H	1.072771	13.312936	7.267974	C	11.396655	6.184669	8.499640
H	2.754347	12.977049	6.772905	H	10.889555	7.125379	8.246294
C	-2.243093	8.640382	6.258579	H	12.397259	6.421593	8.894806
H	-1.757008	7.693038	6.528197	H	11.525216	5.614028	7.566604
H	-3.226083	8.415307	5.815272	C	10.448595	6.173195	10.828176
H	-2.409248	9.207823	7.187626	H	9.900468	5.593336	11.586773
C	-1.169641	8.636631	3.987441	H	11.441607	6.414365	11.238563
H	-0.579993	9.210552	3.255582	H	9.907166	7.112175	10.659916
H	-2.138672	8.391860	3.525147	C	3.970966	2.341359	9.931753
H	-0.636841	7.699886	4.195531	H	3.704271	2.992219	10.777348
C	5.235362	12.465920	5.105438	H	4.119941	1.317116	10.307367
H	5.479453	11.828273	4.243204	H	4.918878	2.722702	9.530858
H	5.087469	13.498150	4.752196	C	3.275129	1.424139	7.704376
H	4.291754	12.086421	5.519547	H	4.211469	1.760298	7.235308
C	5.969494	13.329306	7.338978	H	3.425687	0.397304	8.075132
H	5.037369	12.984569	7.811533	H	2.498334	1.395005	6.925730
H	5.816930	14.364988	6.994672	H	4.927936	5.786284	6.002280
H	6.755438	13.339055	8.108792	H	0.051215	7.809891	8.639680
Mn	3.749603	6.516160	8.296305	H	4.339296	8.973266	8.883735
Mn	6.813153	6.418487	7.733651	H	8.217629	5.598207	5.695565

**Table S16.** Cartesian coordinates of the H-substituted **3-iEt**.

Total Energy: -7684.519785911066 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	5.615971	8.286633	6.485563	O	5.218366	6.315879	6.737026
Mn	2.267772	8.455968	7.197288	O	5.484737	6.221836	9.507635
O	4.034804	8.482154	8.192471	O	2.162348	6.390769	7.127614
O	3.768233	8.575182	5.422043	O	2.634337	6.686717	10.303383
O	7.090432	8.406509	7.803514	O	3.461030	4.547284	8.724313
O	6.618249	8.108568	4.626030	O	8.679536	6.126182	8.747815
O	5.793212	10.249208	6.204457	O	6.904691	4.388743	7.621206
O	0.573573	8.672053	6.182397	O	8.216325	6.510658	5.987212
O	2.348853	10.409193	7.308160	H	7.771404	7.077744	5.314355
O	1.037424	8.285608	8.941659	C	3.083645	6.170925	11.371929
H	1.482151	7.718133	9.614340	C	2.601534	3.749547	8.285984
C	6.168871	8.624251	3.557412	C	2.055112	6.096181	12.511291
C	6.651814	11.047254	6.643610	C	4.401344	5.726543	11.575282
C	7.197534	8.698949	2.418113	H	4.627776	5.316025	12.555394
C	4.851569	9.069655	3.354250	C	8.960145	3.788820	8.626311
H	4.625455	9.480836	2.374342	H	9.594703	2.943897	8.879520
C	0.293657	11.009501	6.302709	C	9.376445	5.089401	8.954696
H	-0.340672	11.854526	6.049256	C	2.721414	2.293379	8.752424
C	-0.122974	9.708878	5.974882	C	1.416819	5.383521	6.826845
C	6.532410	12.503231	6.176356	C	5.509451	5.797053	10.699695
C	7.835487	9.414073	8.104437	C	1.584760	4.112142	7.365336
C	3.743658	9.000405	4.230226	H	0.894916	3.341664	7.025115
C	7.667814	10.685205	7.565426	C	10.751852	5.339301	9.592809
H	8.357095	11.455967	7.906164	C	2.527076	5.303478	13.728172
C	-1.498418	9.459082	5.336636	H	3.395785	5.770327	14.215814
C	6.725364	9.490741	1.200711	H	1.717836	5.257189	14.473375
H	5.857081	9.023075	0.713087	H	2.794655	4.270089	13.460076
H	7.534780	9.537193	0.455693	C	1.752064	7.539440	12.937064
H	6.457042	10.524095	1.468218	H	1.416763	8.142041	12.081978
C	7.501371	7.255605	1.993153	H	0.961030	7.556536	13.703307
H	7.837113	6.653720	2.848547	H	2.648583	8.021571	13.356720
H	8.292336	7.238518	1.226833	C	7.727062	3.514094	8.001870
H	6.605082	6.772727	1.573878	C	0.792092	5.434214	11.944426
C	1.526696	11.283917	6.927371	H	0.999413	4.396743	11.638204
C	8.460137	9.361912	2.984747	H	-0.004752	5.414930	12.704106
H	8.252256	10.399526	3.290161	H	0.425623	5.971809	11.060387
H	9.257125	9.381020	2.225202	C	11.511340	4.056098	9.924148
H	8.826660	8.825128	3.869253	H	11.718081	3.457694	9.024423
C	-2.257175	10.742374	5.004033	H	12.479893	4.308520	10.382788
H	-2.464156	11.341425	5.903273	H	10.958130	3.427646	10.638393
H	-3.225578	10.490135	4.544962	C	0.359951	5.632144	5.803175

H	-1.703209	11.370138	4.289762	H	0.843755	5.843012	4.835399
C	8.891316	9.166067	9.129373	H	-0.309834	4.771761	5.688342
H	8.406610	8.955216	10.096686	H	-0.198754	6.537752	6.069473
H	9.560627	10.026744	9.244720	C	1.370180	1.771824	9.251992
H	9.450621	8.260633	8.863752	H	0.606436	1.762921	8.461092
C	7.883903	13.023531	5.676130	H	1.479537	0.739644	9.620943
H	8.647897	13.032073	6.466807	H	0.990345	2.389728	10.080340
H	7.775279	14.055643	5.306757	C	6.845454	5.359508	11.219577
H	8.262952	12.404960	4.847907	H	7.568579	6.174737	11.077348
C	2.407930	9.439182	3.710625	H	6.814334	5.066573	12.275722
H	1.684221	8.624408	3.852554	H	7.213759	4.515224	10.616504
H	2.439118	9.732594	2.654620	C	7.322094	2.084867	7.762531
H	2.040316	10.283459	4.314120	H	6.958229	1.976631	6.730236
C	1.931654	12.713096	7.167238	H	8.140905	1.377069	7.943782
H	2.295469	12.820927	8.199612	H	6.481625	1.831011	8.427348
H	1.112869	13.420993	6.986124	C	11.571586	6.154252	8.581691
H	2.772218	12.967148	6.502567	H	11.056970	7.086041	8.310014
C	-2.318793	8.645398	6.348267	H	12.556174	6.409985	9.003955
H	-1.804443	7.713827	6.621219	H	11.737328	5.578622	7.657487
H	-3.303211	8.389366	5.925777	C	10.554630	6.147323	10.880249
H	-2.484947	9.222090	7.271746	H	10.005152	5.559800	11.631999
C	-1.301277	8.649788	4.049978	H	11.530062	6.421621	11.311558
H	-0.751212	9.236335	3.297909	H	9.988764	7.067354	10.686436
H	-2.276743	8.375761	3.618587	C	3.746725	2.211568	9.882254
H	-0.736092	7.729568	4.244846	H	3.434172	2.813474	10.748231
C	5.506925	12.584659	5.046694	H	3.870368	1.165872	10.204099
H	5.818958	11.982001	4.181056	H	4.718466	2.607672	9.559104
H	5.383597	13.630185	4.724197	C	3.202380	1.459411	7.556003
H	4.535121	12.189141	5.370427	H	4.160959	1.843901	7.174406
C	6.052068	13.338387	7.372178	H	3.349130	0.409558	7.857097
H	5.093230	12.954795	7.754075	H	2.476745	1.479002	6.729062
H	5.905992	14.388103	7.070291	H	4.182804	9.083447	8.968738
H	6.777684	13.319008	8.199124	H	5.070550	5.714693	5.960640
Mn	3.638303	6.508615	8.444086	H	8.371087	5.607227	5.605230
Mn	6.986025	6.341378	7.732973	H	0.167041	7.878265	8.691552

**Table S17.** Cartesian coordinates of the H-substituted **3-iPr**.

Total Energy: -7684.497806268972 Hartree

Atom	X	Y	Z	Atom	X	Y	Z
Mn	5.192058	8.161238	6.624993	O	5.160284	6.188841	6.721936
Mn	2.158313	8.765053	7.131288	O	5.753596	6.217329	9.326672
O	4.077214	8.599918	8.214256	O	2.267357	6.749475	7.360143
O	3.494368	8.579166	5.599938	O	2.969825	6.792734	9.982675
O	6.978569	8.049573	7.573382	O	3.810699	4.735110	8.596801
O	6.265335	7.947487	4.940064	O	8.848458	5.861091	8.745193
O	5.447376	10.053762	6.318522	O	6.971508	4.090822	7.790576
O	0.404545	8.944460	6.170613	O	8.232382	6.222475	6.028558
O	2.288532	10.703182	7.130832	H	7.762804	6.784227	5.378986
O	1.005320	8.591914	8.879123	C	3.329030	6.265866	11.083483
H	1.450468	8.007625	9.525771	C	2.786992	4.032021	8.414141
C	5.922153	8.494015	3.844703	C	2.220021	6.123011	12.139136
C	6.463766	10.763817	6.518094	C	4.622216	5.819022	11.375482
C	7.050002	8.636456	2.810643	H	4.794757	5.412253	12.367225
C	4.636769	8.961864	3.549804	C	9.093365	3.516978	8.681184
H	4.474063	9.377685	2.560089	H	9.735324	2.674146	8.923467
C	0.167464	11.290822	6.245590	C	9.520331	4.818870	8.995821
H	-0.470940	12.137292	6.006249	C	2.940184	2.552035	8.784197
C	-0.264106	9.991274	5.924536	C	1.398532	5.803311	7.333305
C	6.303971	12.248701	6.162645	C	5.746895	5.810133	10.531812
C	7.848318	8.993898	7.606520	C	1.601876	4.513892	7.832622
C	3.507635	8.980845	4.390184	H	0.770635	3.823443	7.719079
C	7.646805	10.284370	7.110512	C	10.889936	5.058247	9.655496
H	8.474374	10.977796	7.235683	C	2.653444	5.367278	13.394208
C	-1.633210	9.760118	5.259023	H	3.453668	5.892416	13.937451
C	6.637762	9.376418	1.539722	H	1.794539	5.274860	14.077140
H	5.848982	8.842217	0.987908	H	3.002858	4.352007	13.159914
H	7.508537	9.464089	0.872065	C	1.769493	7.528485	12.546586
H	6.280261	10.395105	1.756240	H	1.439893	8.109299	11.677163
C	7.531077	7.230365	2.426202	H	0.929608	7.475676	13.257107
H	7.845567	6.658727	3.308284	H	2.592154	8.083958	13.023239
H	8.388598	7.289487	1.737394	C	7.842716	3.227560	8.107398
H	6.729225	6.659450	1.929754	C	1.065511	5.353380	11.481769
C	1.421030	11.572762	6.817588	H	1.371691	4.323563	11.246203
C	8.178981	9.420487	3.496171	H	0.196716	5.305603	12.155944
H	7.856627	10.451173	3.713631	H	0.760706	5.820396	10.538181
H	9.067047	9.469282	2.845900	C	11.540003	3.779232	10.178371
H	8.459822	8.962439	4.453029	H	11.781013	3.075184	9.368380
C	-2.292820	11.046916	4.771816	H	12.483821	4.025983	10.688428
H	-2.534185	11.727883	5.600328	H	10.891469	3.262850	10.901822
H	-3.237442	10.807207	4.258881	C	0.114475	6.085818	6.644596

H	-1.650717	11.585583	4.059308	H	0.310946	6.301840	5.586818
C	9.150919	8.696836	8.278773	H	-0.578026	5.242907	6.724784
H	8.961229	8.459134	9.337902	H	-0.331519	6.999146	7.039740
H	9.845149	9.543677	8.216127	C	1.609193	1.862148	9.081282
H	9.600778	7.790753	7.853494	H	0.960494	1.805407	8.194643
C	7.629492	12.934288	5.845207	H	1.793171	0.829675	9.413670
H	8.294784	12.979244	6.718400	H	1.054214	2.378918	9.878439
H	7.442706	13.971845	5.524568	C	7.037288	5.302206	11.087866
H	8.166497	12.419935	5.033170	H	7.805355	6.080750	10.983310
C	2.224695	9.491369	3.820355	H	6.943368	5.013195	12.140833
H	1.455066	8.712955	3.916652	H	7.390830	4.440650	10.503195
H	2.330609	9.778553	2.767493	C	7.457876	1.793725	7.869217
H	1.865517	10.354601	4.399829	H	7.093522	1.675752	6.837573
C	1.815490	13.004187	7.057435	H	8.288308	1.098892	8.047297
H	2.188048	13.117086	8.086783	H	6.620594	1.526382	8.533157
H	0.987385	13.704370	6.887367	C	11.806885	5.689731	8.599202
H	2.649526	13.269610	6.388330	H	11.378273	6.624410	8.212772
C	-2.546656	9.093497	6.295813	H	12.790803	5.920647	9.036233
H	-2.111087	8.153755	6.657507	H	11.965307	5.004415	7.752860
H	-3.528563	8.866395	5.852037	C	10.709938	6.035832	10.820117
H	-2.711402	9.754258	7.159287	H	10.097704	5.591236	11.618248
C	-1.447859	8.817852	4.068265	H	11.687876	6.299040	11.251244
H	-0.840846	9.288546	3.283151	H	10.217082	6.955954	10.483627
H	-2.424283	8.558127	3.630771	C	3.866225	2.444402	9.997292
H	-0.947671	7.893631	4.379272	H	3.424934	2.921344	10.883843
C	5.357467	12.375723	4.969575	H	4.054498	1.387074	10.231982
H	5.780230	11.903382	4.069917	H	4.819434	2.949314	9.795618
H	5.168333	13.438606	4.748115	C	3.614965	1.886136	7.575375
H	4.407450	11.873827	5.185209	H	4.575671	2.377150	7.360554
C	5.654873	12.909418	7.388330	H	3.803857	0.821068	7.781236
H	4.697275	12.423623	7.615031	H	2.981940	1.954704	6.677244
H	5.467062	13.978599	7.194452	H	4.360540	9.196226	8.956005
H	6.301661	12.829408	8.273775	H	0.118289	8.209356	8.649180
Mn	4.057440	6.636149	8.302997	H	8.382888	5.323000	5.635695
Mn	7.089929	6.030336	7.788222	H	4.872350	5.591365	5.982907

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