

Electronic Supplementary Information for Dalton Transactions
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**Theoretical magnetochemistry of dinuclear manganese complexes:
broken symmetry density functional theory investigation on the
influence of bridging motifs on structure and magnetism**

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ELECTRONIC SUPPLEMENTARY INFORMATION

Cartesian coordinates of dinuclear manganese models

(μ -O)	IV-IV		
O	-0.013401	0.361402	0.278020
Mn	-0.004157	0.280755	2.284713
Mn	0.005962	0.409985	-1.729544
N	-0.549040	2.315328	2.593167
H	0.238067	2.986452	2.544790
H	-0.992883	2.512784	3.509815
H	-1.236457	2.653958	1.902049
N	-2.069482	-0.175841	2.519139
H	-2.539312	0.351044	3.279362
H	-2.273719	-1.168665	2.735984
H	-2.624062	0.036496	1.676022
N	0.097658	0.120840	4.462061
H	0.189501	1.027873	4.957309
H	0.907064	-0.435791	4.796367
H	-0.727929	-0.331056	4.898927
N	0.432662	-1.798750	2.346637
H	0.118834	-2.285411	3.207399
H	1.438650	-2.033744	2.279826
H	-0.015749	-2.316263	1.575315
N	1.218858	2.147067	-1.922625
H	2.206850	1.962115	-2.175904
H	1.262097	2.703374	-1.055316
H	0.893611	2.816693	-2.645224
N	-1.291238	-1.258308	-1.991004
H	-0.817982	-2.148295	-2.231206
H	-1.849915	-1.469525	-1.150866
H	-1.988164	-1.138808	-2.750109
N	0.055462	0.348111	-3.915245
H	0.247230	-0.598434	-4.294608
H	-0.829758	0.633349	-4.375022
H	0.779109	0.953947	-4.346426
N	-1.668326	1.708098	-1.936863
H	-1.707796	2.227854	-2.833855
H	-2.589400	1.238961	-1.876649
H	-1.692181	2.446671	-1.216551
N	1.750762	-0.793609	-1.894364
H	2.305600	-0.642281	-2.757797
H	1.576653	-1.814119	-1.885882
H	2.416263	-0.628955	-1.123841
N	2.042894	0.820698	2.509619
H	2.223570	1.485524	3.285267
H	2.434169	1.278801	1.673210
H	2.684081	0.031568	2.709875

(μ-O)	III-III		
O	-0.019951	0.373379	0.280031
Mn	0.003178	0.288689	2.192129
Mn	-0.003236	0.402272	-1.636833
N	-0.568872	2.406864	2.512382
H	0.208143	3.076857	2.443243
H	-0.994641	2.598861	3.429774
H	-1.261434	2.728463	1.826611
N	-2.145626	-0.198371	2.416632
H	-2.616419	0.308025	3.179269
H	-2.350910	-1.189462	2.601383
H	-2.675993	0.036171	1.570230
N	0.099932	0.120886	4.528247
H	0.211808	1.011481	5.032837
H	0.885060	-0.449609	4.872406
H	-0.724269	-0.307384	4.972748
N	0.481239	-1.870726	2.255730
H	0.072982	-2.375589	3.054587
H	1.484223	-2.093670	2.299137
H	0.135305	-2.354615	1.419821
N	1.269550	2.204654	-1.817850
H	2.256299	2.019717	-2.042987
H	1.286163	2.744061	-0.945218
H	0.961321	2.869460	-2.540846
N	-1.358070	-1.330054	-1.900207
H	-0.895027	-2.209621	-2.165401
H	-1.885090	-1.549810	-1.047839
H	-2.068304	-1.190283	-2.632185
N	0.052508	0.348626	-3.982556
H	0.258943	-0.581707	-4.372699
H	-0.822511	0.617269	-4.454231
H	0.759213	0.957070	-4.419227
N	-1.744298	1.759390	-1.853458
H	-1.785510	2.256570	-2.753921
H	-2.660754	1.300615	-1.769771
H	-1.749588	2.499549	-1.142410
N	1.801798	-0.867561	-1.807495
H	2.405696	-0.645532	-2.611041
H	1.617417	-1.875167	-1.898819
H	2.402396	-0.779313	-0.980458
N	2.133113	0.856864	2.419610
H	2.298946	1.550703	3.161786
H	2.523212	1.272262	1.566518
H	2.766713	0.081608	2.656312

(μ -O)₂ IV-IV

O	1.292359	0.015839	1.500665
Mn	0.043401	0.011800	2.869069
O	-1.101060	0.003814	1.419287
Mn	0.147254	0.006845	0.051782
N	0.036788	-2.068265	3.155162
N	-1.608840	0.008145	4.262632
N	0.046288	2.093282	3.150206
N	1.616123	0.023560	4.362912
N	-1.425308	0.006433	-1.440058
N	1.808405	0.008669	-1.337602
N	0.184776	-2.073674	-0.234858
N	0.129833	2.086817	-0.247195
H	0.187678	2.348366	-1.243876
H	-0.731346	2.538037	0.092394
H	0.925803	2.563985	0.198615
H	0.278334	-2.336831	-1.228507
H	0.978626	-2.531418	0.234154
H	-0.675615	-2.540132	0.085896
H	1.599573	-0.179950	-2.330811
H	2.337806	0.893398	-1.341038
H	2.514602	-0.692733	-1.066448
H	-1.777751	-0.924271	-1.709260
H	-2.253796	0.480634	-1.047649
H	-1.234466	0.475133	-2.339332
H	-0.079586	-2.337472	4.144644
H	-0.735287	-2.539267	2.663845
H	0.915187	-2.515495	2.856185
H	-0.047740	2.367444	4.140551
H	0.920123	2.536583	2.832759
H	-0.733345	2.565724	2.672282
H	1.785015	-0.861855	4.863536
H	2.505696	0.221678	3.877508
H	1.552153	0.724733	5.116711
H	-1.380736	-0.080766	5.265561
H	-2.193291	0.854943	4.193461
H	-2.271460	-0.756698	4.062665

(μ -O)₂ III-IV

O	1.312678	0.034155	1.657589
Mn	0.046654	0.018865	2.935179
O	-1.129634	-0.009928	1.574624
Mn	0.141742	0.004669	0.161981
N	0.080541	-2.063369	3.081833
N	-1.589697	-0.012836	4.375085
N	0.003884	2.101865	3.062349
N	1.584683	0.061734	4.480067
N	-1.471381	-0.033865	-1.260031

N	1.853795	0.031560	-1.139651
N	0.210193	-2.436767	-0.425852
N	0.116620	2.439330	-0.449855
H	0.143771	2.567946	-1.469914
H	-0.717927	2.964432	-0.160582
H	0.910918	2.997852	-0.113621
H	0.255946	-2.573346	-1.444201
H	1.020615	-2.961049	-0.073399
H	-0.607333	-2.991197	-0.142686
H	1.693659	0.043975	-2.154919
H	2.443342	0.848496	-0.937960
H	2.459058	-0.779108	-0.960742
H	-2.066980	-0.857148	-1.108118
H	-2.095498	0.770287	-1.120590
H	-1.236850	-0.037709	-2.260806
H	0.037516	-2.471959	4.023886
H	-0.714704	-2.447272	2.558766
H	0.940507	-2.415641	2.645838
H	-0.014456	2.517654	4.002072
H	0.831720	2.482177	2.589602
H	-0.825586	2.450985	2.568533
H	1.707248	-0.792581	5.038507
H	2.475547	0.189992	3.980282
H	1.540855	0.816834	5.176360
H	-1.589800	-0.760989	5.080186
H	-1.749159	0.846744	4.915842
H	-2.446291	-0.147754	3.820192

(μ -O)₂ III-III

O	1.340299	0.014276	1.499681
Mn	0.053571	0.015468	2.837546
O	-1.142698	0.003406	1.417619
Mn	0.144068	0.002976	0.079800
N	-0.348238	-2.422833	3.237801
N	-1.615146	0.242541	4.200748
N	0.434420	2.459756	3.238269
N	1.622889	-0.193880	4.316571
N	-1.423905	-0.229083	-1.396892
N	1.809829	0.227632	-1.287416
N	0.559241	-2.436776	-0.297410
N	-0.248767	2.441545	-0.343224
H	-0.459659	2.846338	-1.262232
H	-1.092742	2.575991	0.222280
H	0.471353	3.049736	0.058249
H	0.825418	-2.849767	-1.198231
H	1.365933	-2.569330	0.320558
H	-0.186712	-3.039113	0.063693

H	1.920865	-0.464142	-2.035117
H	1.861901	1.147773	-1.735114
H	2.635575	0.150559	-0.682032
H	-1.450232	-1.153849	-1.837317
H	-2.290346	-0.141053	-0.852991
H	-1.477065	0.454740	-2.158133
H	-0.613579	-2.830391	4.141339
H	-1.153640	-2.563531	2.619956
H	0.401012	-3.024132	2.881865
H	0.644214	2.873098	4.153701
H	1.277867	2.591591	2.671377
H	-0.287599	3.062211	2.831599
H	1.658395	-1.118350	4.756984
H	2.489669	-0.096188	3.774952
H	1.666042	0.490292	5.078147
H	-1.717567	-0.434716	4.962850
H	-1.678621	1.171148	4.629136
H	-2.439849	0.143097	3.597236

(μ -O)₃ IV-IV

O	1.266341	-0.239788	1.357215
Mn	0.023409	-0.133349	2.735298
O	-0.192882	-1.935792	2.337859
Mn	-0.079739	-1.274472	0.606757
O	-1.158017	0.062585	1.318847
N	1.511345	-0.568197	4.187906
N	-1.568147	-0.184367	4.140310
N	0.285666	1.968666	2.891155
N	-1.772403	-2.404400	0.000787
N	1.307981	-2.782630	0.049365
N	0.078148	-0.249114	-1.246981
H	-1.797981	-2.893775	-0.900460
H	-1.935382	-3.104476	0.734257
H	-2.579307	-1.769708	0.027578
H	0.972035	0.256256	-1.231906
H	0.023395	-0.747447	-2.142000
H	-0.655342	0.469700	-1.251716
H	1.263927	-3.243989	-0.865867
H	2.241909	-2.364365	0.136678
H	1.256513	-3.517292	0.765088
H	0.359217	2.435748	3.801555
H	1.136775	2.193841	2.362259
H	-0.490823	2.408442	2.383009
H	1.541036	-0.083317	5.091474
H	1.446460	-1.574479	4.382584
H	2.420784	-0.423949	3.733142
H	-1.510246	0.315301	5.034401

H	-2.404139	0.157562	3.651649
H	-1.746121	-1.173022	4.353642

	(μ-O)(μ-OAc)	IV-IV	
Mn	0.660126	2.430665	0.214521
Mn	0.906169	2.481023	3.743651
O	0.596011	3.061663	1.982779
O	1.233120	0.713265	0.830581
O	1.384467	0.744908	3.105807
C	1.490280	0.130198	1.964068
C	1.912452	-1.291518	1.955796
H	2.600300	-1.511788	2.788294
H	1.017034	-1.933176	2.115432
H	2.348119	-1.580554	0.987788
N	0.008846	4.286332	-0.586019
H	0.759702	4.887496	-0.964441
H	-0.680530	4.224185	-1.354621
H	-0.444423	4.855690	0.146104
N	0.796199	1.569597	-1.763616
H	0.683239	2.204193	-2.572879
H	1.709187	1.104409	-1.900985
H	0.113316	0.809075	-1.918059
N	0.414196	4.374653	4.570395
H	1.103802	4.761379	5.236946
H	-0.483594	4.414209	5.081424
H	0.329018	5.080289	3.821782
N	1.291005	1.674008	5.709976
H	1.091711	2.279267	6.525092
H	2.273034	1.373145	5.826428
H	0.753361	0.805974	5.872636
N	2.634046	3.061906	-0.174794
H	2.806371	3.314085	-1.163161
H	3.326169	2.323723	0.031163
H	2.915576	3.894209	0.363495
N	-1.362554	1.845072	0.120226
H	-1.786892	1.942673	-0.817957
H	-1.489172	0.849616	0.364274
H	-1.978698	2.387577	0.742637
N	-1.084744	1.910244	4.137116
H	-1.359437	2.003302	5.130048
H	-1.257757	0.917863	3.910466
H	-1.782000	2.462414	3.616813
N	2.914535	3.118578	3.827437
H	3.108813	3.941620	3.238669
H	3.569853	2.376401	3.534266
H	3.233128	3.391238	4.772918

(μ-O)(μ-OAc)		III-IV	
Mn	0.625615	2.442974	0.197147
O	0.556568	3.102805	1.844789
O	1.385681	0.744757	3.012485
H	1.009907	-1.920976	2.056324
H	0.631127	5.057146	-0.382063
H	-0.128894	4.328013	-1.644197
N	0.722257	1.591014	-1.819004
H	1.035602	0.614029	-1.714649
H	-0.157740	1.534221	-2.352281
N	0.385508	4.428931	4.454480
H	1.157415	4.920244	4.926756
H	-0.391525	4.426254	5.130206
H	0.086971	5.050633	3.690837
H	1.201150	2.352137	6.444611
H	2.271417	1.360479	5.690027
H	0.713362	0.906283	5.836294
N	-1.361826	1.873732	4.229829
H	-1.570874	1.935709	5.236789
H	-1.575637	0.893678	4.000898
H	-2.118390	2.421654	3.800289
N	3.198824	3.243819	3.839750
H	3.458206	4.097293	3.328352
H	3.873754	2.530687	3.532170
H	3.492781	3.451853	4.805062
Mn	0.899436	2.515226	3.683013
O	1.209876	0.707164	0.741686
C	1.478091	0.142404	1.893437
C	1.897913	-1.289819	1.860975
H	2.619598	-1.498910	2.662852
H	2.302900	-1.573939	0.882468
N	-0.014071	4.290460	-0.620285
H	-0.918267	4.585013	-0.224637
H	1.387208	2.016694	-2.481316
N	1.308882	1.722244	5.636756
N	2.607042	3.023950	-0.134327
H	2.784167	3.537209	-1.010390
H	3.225982	2.200512	-0.161679
H	2.946490	3.629000	0.622536
N	-1.364062	1.798567	0.192023
H	-1.928399	2.089991	-0.619737
H	-1.412280	0.769391	0.211714
H	-1.865246	2.137250	1.021696
(μ-O)(μ-OAc)		III-III	
Mn	0.660520	2.444122	0.288374
Mn	0.898716	2.495807	3.668965

O	0.577859	3.140121	1.982774
O	1.293368	0.654042	0.834829
O	1.378794	0.666677	3.100107
C	1.514494	0.084369	1.963946
C	1.937220	-1.355751	1.955976
H	2.543802	-1.592636	2.837342
H	1.033386	-1.987334	1.993997
H	2.474027	-1.602849	1.033089
N	-0.048754	4.342785	-0.499963
H	0.696498	4.958616	-0.846660
H	-0.743866	4.297207	-1.254854
H	-0.495062	4.851858	0.271505
N	0.780426	1.630964	-1.709259
H	1.152981	2.238633	-2.448370
H	1.408938	0.818593	-1.656352
H	-0.106089	1.264358	-2.074996
N	0.434191	4.459924	4.483248
H	1.066118	4.813561	5.211733
H	-0.512521	4.546729	4.871867
H	0.481890	5.133424	3.710159
N	1.251040	1.725676	5.655764
H	0.650401	2.066213	6.415841
H	2.214371	1.850487	5.988270
H	1.112287	0.707800	5.608436
N	2.908085	3.143362	-0.191056
H	3.153263	3.380397	-1.160440
H	3.565387	2.397391	0.064808
H	3.191201	3.964513	0.354104
N	-1.619143	1.692227	0.199430
H	-2.158805	1.839889	-0.662618
H	-1.678800	0.682332	0.375509
H	-2.182199	2.136994	0.931236
N	-1.359374	1.828782	4.145405
H	-1.681123	1.858608	5.120913
H	-1.504656	0.854119	3.857705
H	-2.053140	2.379433	3.628423
N	3.210042	3.143688	3.762318
H	3.422120	3.857129	3.057610
H	3.820321	2.346704	3.545776
H	3.585171	3.530143	4.637608
(μ-O)(μ-OAc)₂			
O	1.441658	2.754416	1.319780
Mn	1.014568	1.919926	2.895722
Mn	2.538913	2.100052	0.006678
O	1.702579	0.372929	0.023939
O	0.648950	0.244481	2.029158

O	2.842332	1.464966	3.266337
O	3.900949	1.586569	1.263582
C	0.980334	-0.262814	0.887407
C	3.903399	1.358232	2.535644
C	5.175677	0.940472	3.183005
C	0.525567	-1.640195	0.559791
H	-0.397918	-1.896062	1.096340
H	0.408660	-1.775633	-0.524279
H	1.309653	-2.349103	0.894675
H	5.230631	-0.166382	3.150817
H	6.047838	1.326799	2.638279
H	5.202588	1.237064	4.240445
N	1.223022	2.666459	-1.525302
N	3.833236	1.269814	-1.467522
N	3.533852	3.933516	-0.220911
H	1.654450	3.001869	-2.399550
H	0.637781	1.861579	-1.795299
H	0.578043	3.409583	-1.220517
H	3.039693	4.688226	0.275800
H	4.475634	3.874898	0.195418
H	3.672149	4.271801	-1.184923
H	3.424850	0.396956	-1.835246
H	4.101350	1.829938	-2.290008
H	4.716612	0.996310	-1.010588
N	-1.022732	2.383466	2.717420
H	-1.489405	2.751172	3.559955
H	-1.182386	3.080833	1.976683
H	-1.552213	1.540306	2.448276
N	1.278921	3.675975	4.012350
H	1.207053	4.516849	3.421818
H	2.223890	3.685119	4.424904
H	0.630838	3.822770	4.800682
N	0.577403	0.886539	4.706628
H	1.447340	0.749591	5.243583
H	0.239805	-0.059782	4.472999
H	-0.109799	1.276812	5.368087

	(μ-O)(μ-OAc)₂	III-IV	
Mn	0.965486	1.989064	2.914059
O	1.715174	0.321904	0.032106
O	3.926513	1.546967	1.278642
C	3.941052	1.329168	2.568136
C	5.254727	0.892567	3.147296
C	0.561894	-1.711562	0.500420
H	-0.377074	-1.989864	0.992533
H	0.484716	-1.820083	-0.587359
H	1.346656	-2.404282	0.850606

H	5.286545	-0.210660	3.128393
H	6.101300	1.260801	2.557331
H	5.335667	1.209775	4.193683
N	1.184300	2.620882	-1.483659
N	3.536127	3.919060	-0.161320
H	1.579533	3.023331	-2.342599
H	0.654121	1.788782	-1.772737
H	0.501085	3.299168	-1.126240
H	3.006824	4.659710	0.313874
H	4.449498	3.858909	0.307004
H	3.721620	4.254536	-1.114739
N	0.529884	0.959407	4.694817
H	1.415892	0.756369	5.177556
H	0.117111	0.048158	4.453003
H	-0.092767	1.393330	5.386850
O	1.433464	2.780039	1.301284
Mn	2.523647	2.062175	0.072359
O	0.597272	0.164789	1.996574
O	2.926611	1.451138	3.309913
C	0.964542	-0.319639	0.890364
N	3.825069	1.234939	-1.423437
H	3.429106	0.333919	-1.722428
H	4.057283	1.752904	-2.279669
H	4.717914	1.013211	-0.963160
N	-1.196611	2.470293	2.665841
H	-1.710939	2.790534	3.495769
H	-1.332028	3.203395	1.960171
H	-1.709128	1.647990	2.323333
N	1.326278	3.855541	4.085774
H	1.348896	4.678750	3.472958
H	2.246118	3.815831	4.542304
H	0.658039	4.087738	4.831021
(μ-O)(μ-OAc)₂			
O	1.402580	2.819799	1.303973
Mn	1.030409	1.936261	2.844433
Mn	2.504394	2.111038	0.048916
O	1.615166	0.240494	-0.025939
O	0.557474	0.113388	1.965230
O	2.997590	1.454651	3.339217
O	4.057863	1.592513	1.350669
C	0.899240	-0.379101	0.835516
C	4.043805	1.359532	2.608083
C	5.329317	0.923975	3.265037
C	0.453827	-1.781580	0.508830
H	-0.486175	-2.024501	1.016833
H	0.358190	-1.923307	-0.573476

H	1.222196	-2.482668	0.872337
H	5.379150	-0.176276	3.235217
H	6.199850	1.312597	2.724932
H	5.357594	1.229398	4.317118
N	1.066150	2.680782	-1.632622
N	3.811658	1.228632	-1.374057
N	3.594929	4.083228	-0.182965
H	1.404484	3.120916	-2.494390
H	0.569181	1.829583	-1.916144
H	0.359914	3.312922	-1.243509
H	3.036875	4.815773	0.266088
H	4.467236	4.010612	0.351751
H	3.849097	4.438975	-1.110136
H	3.404055	0.316671	-1.613137
H	4.043433	1.705707	-2.250302
H	4.690621	1.042513	-0.876005
N	-1.185084	2.422116	2.656359
H	-1.728501	2.731784	3.468541
H	-1.294117	3.147795	1.941313
H	-1.653419	1.584350	2.294728
N	1.370374	3.815377	4.078460
H	1.425977	4.611425	3.435851
H	2.293522	3.729564	4.517150
H	0.718056	4.087570	4.820899
N	0.633026	0.849666	4.626255
H	1.549457	0.651981	5.046228
H	0.236450	-0.051963	4.335309
H	0.029919	1.234125	5.359462

(μ-O)(μ-OAc)₃	IV-IV		
Mn	1.292410	-2.698143	-3.312536
Mn	3.184624	-2.397229	-1.014761
O	1.529828	-2.799240	-1.547580
O	2.928700	-2.172213	-4.243598
C	4.087984	-1.892344	-3.776507
O	4.336679	-1.929086	-2.519429
C	5.184907	-1.522979	-4.719537
H	4.793869	-1.343456	-5.727010
H	5.914233	-2.349913	-4.756396
H	5.716197	-0.634195	-4.349085
O	2.089852	-4.495294	-3.284114
C	2.947255	-4.956710	-2.429676
O	3.551485	-4.257439	-1.519260
C	3.295167	-6.407741	-2.517974
H	4.354449	-6.502686	-2.810016
H	2.666506	-6.918941	-3.255251
H	3.191687	-6.879472	-1.529060

O	2.530994	-0.550955	-1.161887
C	1.619155	-0.108716	-1.969794
O	1.086471	-0.781148	-2.941995
C	1.147710	1.295224	-1.768905
H	1.937577	1.907050	-1.314996
H	0.287323	1.279341	-1.076605
H	0.810480	1.729001	-2.718936
N	0.628567	-2.699024	-5.334482
H	-0.238369	-2.185059	-5.540348
H	1.372745	-2.245298	-5.881101
H	0.521010	-3.645003	-5.726774
N	-0.671572	-3.269343	-2.902847
H	-0.972201	-4.106643	-3.420591
H	-0.754928	-3.491102	-1.903140
H	-1.350966	-2.521486	-3.101026
N	2.473296	-2.786708	0.905855
H	2.417380	-1.938175	1.486499
H	3.036401	-3.477388	1.420876
H	1.521074	-3.166857	0.840259
N	5.012903	-1.984504	-0.008265
H	5.634505	-1.560388	-0.709887
H	5.495716	-2.828652	0.330136
H	4.968456	-1.324028	0.779148

	(μ-O)(μ-OAc)₃	III-III	
Mn	1.208873	-2.744992	-3.201044
Mn	3.061672	-2.448507	-0.947189
O	1.379524	-2.869124	-1.417238
O	3.069655	-2.122240	-4.369652
C	4.212103	-1.839354	-3.888584
O	4.474937	-1.880194	-2.644159
C	5.328821	-1.450430	-4.839007
H	4.944842	-1.253157	-5.845593
H	6.057826	-2.272913	-4.890730
H	5.859734	-0.568180	-4.458048
O	2.087850	-4.588548	-3.258816
C	2.972409	-5.024960	-2.441374
O	3.532742	-4.354487	-1.503075
C	3.421765	-6.459410	-2.607031
H	4.462331	-6.467388	-2.963441
H	2.790270	-6.989221	-3.327340
H	3.407246	-6.971975	-1.636042
O	2.462288	-0.503513	-1.125907
C	1.595401	-0.060246	-1.959057
O	1.029331	-0.732838	-2.891597
C	1.188785	1.389633	-1.817487
H	2.005460	1.979837	-1.386813

H	0.327517	1.448289	-1.133784
H	0.882127	1.801009	-2.785793
N	0.715438	-2.699217	-5.287698
H	0.009166	-2.015757	-5.572772
H	1.629253	-2.399779	-5.660166
H	0.477313	-3.602474	-5.705893
N	-0.971632	-3.338265	-2.850068
H	-1.311872	-4.185464	-3.312899
H	-0.978363	-3.518408	-1.842252
H	-1.652047	-2.594322	-3.028391
N	2.364089	-2.818061	1.200920
H	2.292003	-1.974564	1.776722
H	2.865104	-3.523426	1.747834
H	1.412304	-3.165771	1.054748
N	4.984507	-2.012735	-0.104626
H	5.484918	-1.770589	-0.973308
H	5.464373	-2.802762	0.334689
H	5.031497	-1.212442	0.531364

	(μ-O)₂(μ-OAc)	IV-IV	
N	-3.478636	1.510634	2.846968
Mn	-2.611872	-0.054355	4.006737
N	-4.371311	-0.135402	5.136789
O	-1.172606	0.023128	2.715856
C	0.085827	0.037479	2.989071
O	0.517382	0.015938	4.202013
Mn	-0.578641	-0.059176	5.793703
O	-1.730937	-1.278297	5.052969
C	1.069126	0.059541	1.868121
O	-1.791987	1.143206	5.127186
N	-3.397706	-1.581666	2.742985
H	2.037840	0.448818	2.202203
H	1.217111	-0.975528	1.512493
H	0.682197	0.645705	1.024451
N	0.768221	-1.589945	6.413287
N	0.682917	1.507785	6.499225
N	-1.477415	-0.138778	7.683073
H	-4.394664	-1.583700	2.491494
H	-2.879219	-1.567540	1.854098
H	-3.203034	-2.498806	3.167897
H	-3.308277	2.407915	3.321942
H	-2.980789	1.569999	1.948179
H	-4.480562	1.489986	2.616953
H	-4.388028	-0.981208	5.721121
H	-4.438565	0.674285	5.766889
H	-5.247088	-0.147300	4.597387
H	1.134631	-1.598741	7.373892

H	0.322477	-2.505834	6.264332
H	1.589934	-1.573482	5.793862
H	-0.833564	-0.137092	8.485213
H	-2.102586	0.665697	7.821077
H	-2.046992	-0.989405	7.778767
H	1.501347	1.574073	5.878829
H	0.185332	2.403922	6.404337
H	1.052973	1.481394	7.458112

(μ-O)₂(μ-OAc)	III-IV		
N	-3.464013	1.544715	2.906603
Mn	-2.708676	-0.058033	4.101845
N	-4.797139	-0.154600	5.275963
O	-1.045079	0.031970	2.565207
C	0.159741	0.045096	2.908364
O	0.555640	0.023503	4.159857
Mn	-0.560738	-0.052012	5.730585
O	-1.704287	-1.297011	5.106012
C	1.261995	0.061510	1.882359
O	-1.770305	1.167393	5.184457
N	-3.381787	-1.617072	2.802183
H	2.195321	0.463633	2.290802
H	1.449117	-0.972978	1.553226
H	0.945699	0.637137	1.004408
N	0.812037	-1.603842	6.332646
N	0.736668	1.526216	6.423024
N	-1.452793	-0.133252	7.639957
H	-4.351136	-1.640165	2.469992
H	-2.774326	-1.587978	1.974289
H	-3.199497	-2.515575	3.263394
H	-3.326806	2.418861	3.426573
H	-2.857228	1.601894	2.079647
H	-4.433874	1.540054	2.575124
H	-4.843667	-0.993796	5.863825
H	-4.891386	0.643129	5.913738
H	-5.663296	-0.163078	4.725869
H	1.214888	-1.652653	7.274182
H	0.327824	-2.493252	6.163115
H	1.595891	-1.570767	5.670563
H	-0.853309	-0.138744	8.471918
H	-2.080220	0.674177	7.718320
H	-2.031539	-0.979293	7.672153
H	1.514848	1.572720	5.755136
H	0.208951	2.400087	6.312894
H	1.145314	1.535255	7.363281

(μ -O)₂(μ -OAc) **III-III**

N	-3.325380	1.566349	2.863414
Mn	-2.682764	-0.060348	4.118862
N	-4.825318	-0.151173	5.247367
O	-1.005561	0.031210	2.516300
C	0.234725	0.050361	2.816501
O	0.690199	0.034411	4.008257
Mn	-0.682173	-0.058368	5.876971
O	-1.862221	-1.323339	5.204439
C	1.237200	0.062408	1.671817
O	-1.931484	1.177422	5.279690
N	-3.250153	-1.631973	2.761464
H	2.201680	0.472002	1.993755
H	1.401996	-0.973081	1.335344
H	0.847331	0.628472	0.816886
N	0.735857	-1.632167	6.261181
N	0.647520	1.563498	6.361548
N	-1.531119	-0.154656	8.144533
H	-4.180284	-1.725850	2.347182
H	-2.557497	-1.535798	2.009332
H	-3.031610	-2.495170	3.268332
H	-3.150571	2.402585	3.429103
H	-2.624319	1.553594	2.112992
H	-4.256422	1.643935	2.447825
H	-4.743904	-0.989901	5.828623
H	-4.781081	0.651983	5.880594
H	-5.763320	-0.159318	4.836340
H	1.267822	-1.731268	7.128805
H	0.202201	-2.493126	6.106769
H	1.391309	-1.534539	5.476535
H	-1.006062	-0.172222	9.023652
H	-2.163399	0.649279	8.187339
H	-2.119521	-0.992212	8.128213
H	1.305998	1.553581	5.573509
H	0.068160	2.402850	6.263320
H	1.175002	1.633820	7.234713

	(μ-O)₂(μ-OAc)₂	IV-IV	
Mn	4.462393	0.547576	3.472878
Mn	2.440582	-0.938004	4.104687
O	5.287689	-1.114633	2.815668
O	3.498129	-2.430038	3.376273
O	3.404864	2.039389	4.198607
O	1.614722	0.725756	4.761270
O	2.947915	0.004903	2.652107
O	3.954232	-0.395214	4.925778
N	5.009621	1.632841	1.748721
H	5.069133	2.647550	1.893496

H	4.272020	1.478764	1.050749
H	5.889886	1.326405	1.318193
N	6.214677	1.149568	4.483279
H	6.174378	0.735085	5.422162
H	7.084117	0.814819	4.051706
H	6.302024	2.164158	4.613850
N	0.690242	-1.543037	3.094008
H	-0.183448	-1.240470	3.540429
H	0.713188	-1.103363	2.166044
H	0.625855	-2.555749	2.937345
N	1.893958	-2.020200	5.831589
H	1.040562	-1.674511	6.286142
H	2.656049	-1.904051	6.510282
H	1.781784	-3.030354	5.686420
C	2.223220	1.862147	4.691244
C	4.678810	-2.252332	2.884674
C	5.398886	-3.450989	2.347077
H	4.826772	-4.365526	2.532664
H	5.552525	-3.324617	1.264670
H	6.392738	-3.524337	2.810840
C	1.514570	3.068609	5.226451
H	1.515661	3.865860	4.470055
H	0.488270	2.821529	5.516013
H	2.062243	3.448803	6.102301

	(μ-O)₂(μ-OAc)₂	III-IV	
Mn	4.637407	0.674933	3.420685
Mn	2.588536	-0.828714	4.061039
O	5.395218	-1.395607	2.711608
O	3.472397	-2.436796	3.379846
O	3.215386	2.261544	4.336058
O	1.600547	0.702853	4.772870
O	3.072533	0.107596	2.605862
O	4.091901	-0.305323	4.896231
N	5.114543	1.734949	1.646667
H	5.172176	2.753794	1.737374
H	4.307353	1.527314	1.048142
H	5.951231	1.411708	1.151489
N	6.372175	1.232612	4.505700
H	6.220840	0.762210	5.405032
H	7.260405	0.888722	4.128240
H	6.474737	2.233450	4.699093
N	0.822902	-1.424615	3.027223
H	-0.049130	-1.090260	3.446482
H	0.929518	-0.961080	2.119013
H	0.750007	-2.431269	2.855897
N	2.053229	-1.922302	5.808604

H	1.200564	-1.592298	6.269202
H	2.839484	-1.737820	6.440094
H	1.993124	-2.935453	5.674722
C	2.089244	1.920089	4.771277
C	4.672377	-2.411887	2.851418
C	5.186919	-3.757332	2.381038
H	4.469490	-4.560470	2.579081
H	5.395446	-3.705500	1.303108
H	6.138508	-3.975904	2.885261
C	1.172499	2.973188	5.360234
H	0.995225	3.756574	4.610240
H	0.217136	2.547809	5.684654
H	1.674343	3.449620	6.214184

(μ-O)₂(μ-OAc)₂	III-III		
Mn	4.473495	0.554760	3.469623
Mn	2.424945	-0.950068	4.109805
O	5.450837	-1.391034	2.692895
O	3.661878	-2.707944	3.253882
O	3.239965	2.313589	4.322572
O	1.449273	1.000027	4.885775
O	2.928149	0.009610	2.617594
O	3.969730	-0.405366	4.962207
N	4.904708	1.610783	1.662439
H	4.897220	2.631265	1.719860
H	4.052450	1.301355	1.179454
H	5.717866	1.299399	1.127260
N	6.206156	1.086034	4.602941
H	5.920120	0.559507	5.437559
H	7.098946	0.715264	4.270988
H	6.311724	2.070880	4.854983
N	0.697764	-1.490831	2.972241
H	-0.205483	-1.147376	3.305081
H	0.973848	-0.947698	2.144920
H	0.618108	-2.474750	2.706976
N	1.987139	-1.993568	5.922923
H	1.192416	-1.643264	6.462001
H	2.854924	-1.709529	6.393797
H	1.954071	-3.014165	5.880264
C	2.074656	2.108449	4.801386
C	4.825994	-2.501006	2.775521
C	5.571791	-3.724036	2.221302
H	5.012114	-4.650255	2.400955
H	5.726308	-3.596942	1.139070
H	6.567426	-3.794613	2.682971
C	1.354865	3.349974	5.348792
H	1.362684	4.150360	4.594862

H	0.322017	3.119443	5.637790
H	1.900166	3.728082	6.226982

(μ -OAc)₂ IV-IV

Mn	0.757073	0.329076	3.479564
Mn	0.871131	0.294557	-1.557195
N	0.794812	-1.775652	3.676876
N	-0.835514	0.307702	4.879208
N	0.760439	2.436405	3.652876
N	2.147639	0.367204	5.062871
N	-0.522005	0.269588	-3.138429
N	2.461909	0.300902	-2.957900
N	0.850097	-1.812755	-1.729330
N	0.849290	2.399422	-1.757342
H	1.065628	2.762096	-2.704247
H	-0.073906	2.800474	-1.517394
H	1.536073	2.857496	-1.136277
H	1.034016	-2.188755	-2.677810
H	1.558581	-2.259586	-1.124343
H	-0.063513	-2.213315	-1.455052
H	2.184896	0.402310	-3.952606
H	3.131236	1.070917	-2.779507
H	3.034441	-0.561666	-2.923234
H	-0.397204	-0.485189	-3.838415
H	-1.468004	0.135238	-2.737333
H	-0.575635	1.141819	-3.696154
H	0.583529	-2.141691	4.623664
H	0.109848	-2.237832	3.056755
H	1.720297	-2.169865	3.434297
H	0.572436	2.808891	4.601867
H	1.671134	2.844654	3.380262
H	0.048762	2.877507	3.047637
H	2.211808	-0.506599	5.617018
H	3.092884	0.515336	4.664695
H	2.012223	1.117438	5.765797
H	-0.559544	0.201602	5.873721
H	-1.412501	1.167369	4.848443
H	-1.500565	-0.464842	4.695634
O	-0.670925	0.308655	-0.331241
C	-1.165203	0.334360	0.873189
O	-0.416346	0.321717	1.939059
C	-2.651497	0.361609	0.994587
H	-3.048950	-0.664205	0.827296
H	-3.112960	0.987347	0.212148
H	-2.984782	0.694059	1.986198
O	2.040409	0.298237	-0.013144
C	2.792994	0.298993	1.049996

O	2.300571	0.325748	2.255070
C	4.279230	0.284431	0.925656
H	4.612885	-0.087441	-0.052159
H	4.751689	-0.299038	1.732943
H	4.663170	1.322492	1.042842

(μ -OAc)₂ III-III

Mn	0.909492	0.332913	3.580108
Mn	0.717377	0.294218	-1.658221
N	0.923302	-1.779965	3.636406
N	-0.806025	0.321989	4.829326
N	0.907798	2.445803	3.604686
N	2.342116	0.360410	5.458481
N	-0.715433	0.266508	-3.536400
N	2.432865	0.300990	-2.907597
N	0.716443	-1.818697	-1.680464
N	0.706063	2.407177	-1.717333
H	0.963456	2.831512	-2.619313
H	-0.242043	2.747007	-1.508244
H	1.331685	2.825722	-1.017400
H	0.931058	-2.252718	-2.589053
H	1.377621	-2.225274	-1.006441
H	-0.218533	-2.161059	-1.422763
H	2.218906	0.428420	-3.907432
H	3.096064	1.049154	-2.662938
H	2.986235	-0.565118	-2.853873
H	-0.633953	-0.519063	-4.196509
H	-1.677482	0.204018	-3.177192
H	-0.722618	1.096883	-4.144572
H	0.665407	-2.206070	4.537404
H	0.298740	-2.197810	2.935116
H	1.871943	-2.118515	3.427669
H	0.693846	2.878405	4.514109
H	1.842097	2.789522	3.346332
H	0.245398	2.852653	2.932019
H	2.352238	-0.471863	6.064006
H	3.303972	0.427444	5.099576
H	2.257717	1.143598	6.121049
H	-0.592406	0.187686	5.828333
H	-1.357774	1.189466	4.781356
H	-1.470553	-0.423320	4.579595
O	-0.804991	0.305796	-0.533137
C	-1.245979	0.321167	0.721378
O	-0.500744	0.311407	1.724406
C	-2.749797	0.329038	0.819846
H	-3.132184	-0.685838	0.618331
H	-3.200872	0.988188	0.066973

H	-3.075894	0.628874	1.821528
O	2.127426	0.314464	0.197329
C	2.872741	0.309456	1.200338
O	2.431742	0.324843	2.454839
C	4.376576	0.306922	1.101772
H	4.703678	0.005061	0.101018
H	4.830227	-0.348083	1.856690
H	4.755127	1.323902	1.299920

(μ-OAc)₃	IV-IV		
Mn	0.744623	0.150504	3.573147
Mn	0.166339	-2.000939	-0.105468
N	2.242589	-0.209913	4.996601
N	-0.634468	0.320776	5.144684
N	1.132453	2.203314	3.765503
N	-1.585219	-2.993000	-0.697225
N	1.265867	-3.662157	-0.759971
N	0.310173	-1.206474	-2.041714
H	-1.509995	-3.652680	-1.489610
H	-1.954609	-3.544101	0.094603
H	-2.323208	-2.316134	-0.952531
H	1.294780	-1.010938	-2.287215
H	-0.075201	-1.773928	-2.815138
H	-0.186698	-0.301632	-2.080857
H	1.172584	-3.927269	-1.754832
H	2.273297	-3.492561	-0.606532
H	1.023786	-4.503991	-0.211548
H	1.451185	2.538921	4.689812
H	1.868522	2.480048	3.095475
H	0.295308	2.760729	3.528185
H	2.136373	0.243265	5.919602
H	2.301806	-1.223896	5.185405
H	3.168557	0.076429	4.638363
H	-0.435060	1.024231	5.875426
H	-1.563692	0.564366	4.764459
H	-0.745318	-0.582339	5.634443
O	1.826233	-1.121409	0.297206
C	2.525774	-0.364436	1.077305
O	2.104576	0.072910	2.219122
C	3.889077	0.039769	0.627839
H	4.325906	-0.699304	-0.058928
H	4.561254	0.216958	1.479839
H	3.806714	0.997820	0.072344
O	0.385148	-1.737881	3.553290
C	0.120955	-2.817264	2.892468
O	0.023174	-2.863062	1.603949
C	-0.065927	-4.083148	3.658297

H	0.919216	-4.588064	3.747640
H	-0.738228	-4.778265	3.134599
H	-0.427984	-3.891763	4.678344
O	-0.932815	-0.503395	0.375993
C	-1.280253	0.401949	1.231153
O	-0.672056	0.596656	2.355316
C	-2.457786	1.258788	0.911216
H	-3.370260	0.762906	1.304996
H	-2.594484	1.372763	-0.173906
H	-2.388637	2.242958	1.396128

(μ-OAc)₃	III-IV		
N	2.254922	-0.162805	5.004898
N	-0.620349	0.380994	5.158214
N	1.208844	2.538823	3.742353
H	-1.524717	-3.579505	-1.544191
H	1.199268	-3.882595	-1.773237
H	1.422111	2.943054	4.664828
H	2.012370	2.797217	3.153998
H	0.425296	3.102381	3.385810
H	2.246992	0.383649	5.877775
H	-0.360612	0.957215	5.971472
O	2.142890	0.125980	2.195807
H	4.303222	-0.843212	-0.068306
H	4.614089	0.071917	1.453130
O	0.384937	-1.894177	3.469016
C	0.110874	-2.950156	2.870965
O	-0.704649	0.652729	2.362141
Mn	0.775560	0.295827	3.593773
Mn	0.166523	-2.033826	-0.032535
N	-1.584397	-2.993649	-0.699050
N	1.270949	-3.662309	-0.769546
N	0.330701	-1.131184	-1.965789
H	-1.922340	-3.606218	0.057189
H	-2.324523	-2.298368	-0.871201
H	1.314540	-0.924581	-2.188797
H	-0.047277	-1.643406	-2.775594
H	-0.158987	-0.225616	-1.953992
H	2.268248	-3.485600	-0.581617
H	1.021998	-4.519108	-0.254339
H	2.205766	-1.154881	5.279259
H	3.184863	-0.017257	4.586713
H	-1.501523	0.777337	4.801013
H	-0.845124	-0.556672	5.521171
O	1.835995	-1.203380	0.370114
C	2.544797	-0.401585	1.113024
C	3.920719	-0.076407	0.614986

H	3.871848	0.879419	0.060822
O	-0.014295	-3.028195	1.543370
C	-0.088481	-4.259203	3.579059
H	0.891206	-4.764995	3.655532
H	-0.764644	-4.929563	3.036004
H	-0.455416	-4.085714	4.598433
O	-0.948351	-0.564851	0.452080
C	-1.312023	0.368886	1.282726
C	-2.544311	1.142989	0.924270
H	-3.410860	0.667572	1.420409
H	-2.732549	1.138187	-0.155612
H	-2.478095	2.173105	1.298060

(μ-OAc)₃	III-III		
Mn	0.742655	0.146371	3.567383
Mn	0.168099	-1.997304	-0.096480
N	2.318652	-0.269330	5.034714
N	-0.732312	0.304712	5.185137
N	1.153929	2.297856	3.723373
N	-1.679011	-3.030278	-0.673191
N	1.349139	-3.725831	-0.755778
N	0.315789	-1.123439	-2.102881
H	-1.687096	-3.584231	-1.537621
H	-1.944612	-3.672304	0.083254
H	-2.441781	-2.347810	-0.758286
H	1.273006	-0.786173	-2.260396
H	0.075189	-1.704202	-2.914667
H	-0.295340	-0.299098	-2.146443
H	1.180945	-4.113892	-1.691347
H	2.344319	-3.473871	-0.722796
H	1.222235	-4.500232	-0.093165
H	1.325369	2.703979	4.650629
H	1.981785	2.514674	3.155298
H	0.373835	2.826942	3.315689
H	2.344883	0.279824	5.901812
H	2.251066	-1.254411	5.317773
H	3.238198	-0.155116	4.591883
H	-0.507105	0.877454	6.006946
H	-1.603479	0.685877	4.796754
H	-0.956334	-0.633114	5.538660
O	1.931616	-1.109331	0.278123
C	2.599674	-0.345150	1.055084
O	2.193624	0.119409	2.173868
C	3.980027	0.065868	0.596234
H	4.421919	-0.694450	-0.056663
H	4.635371	0.270485	1.449664
H	3.885405	0.997787	0.014302

O	0.394316	-1.836046	3.602151
C	0.110473	-2.886836	2.933451
O	-0.008829	-2.952895	1.662314
C	-0.074424	-4.170945	3.709263
H	0.904559	-4.673581	3.780092
H	-0.762175	-4.848791	3.192166
H	-0.422541	-3.970714	4.728162
O	-1.004224	-0.425567	0.349266
C	-1.341593	0.452056	1.214855
O	-0.771680	0.645091	2.342183
C	-2.535702	1.319471	0.888551
H	-3.440280	0.816103	1.268605
H	-2.649890	1.443044	-0.193743
H	-2.463297	2.294055	1.383100

(μ -OAc)₄ IV-IV

Mn	1.253275	-1.005300	-0.724411
O	2.450884	0.005476	-1.754804
C	2.198872	1.240057	-2.092955
O	1.117454	1.832796	-1.744456
C	3.216917	1.938385	-2.924725
H	3.167816	3.026796	-2.791925
H	3.014626	1.711132	-3.989616
H	4.226635	1.563776	-2.702589
O	-1.346503	0.229706	0.183956
C	-1.216447	-0.981722	0.581547
O	-0.161977	-1.694873	0.295111
C	-2.267696	-1.628681	1.413419
H	-2.008028	-1.482346	2.480264
H	-2.295069	-2.713400	1.235058
H	-3.253899	-1.180223	1.237152
O	0.239220	2.348003	0.757086
C	1.145739	1.557040	1.262474
O	1.446228	0.434535	0.721870
C	1.839037	2.020669	2.495325
H	2.239910	1.179147	3.074461
H	1.167432	2.634704	3.113011
H	2.685867	2.669262	2.196871
O	-0.124499	-0.699935	-2.210284
C	-1.032621	-0.016286	-2.802430
O	-1.426973	1.144505	-2.355632
C	-1.672029	-0.515268	-4.050587
H	-2.709801	-0.159377	-4.126612
H	-1.629980	-1.609958	-4.115815
H	-1.123030	-0.095963	-4.916331
Mn	-0.701452	1.907093	-0.803287
N	2.728178	-1.854738	0.457588

H	3.625279	-1.998307	-0.032220
H	2.897931	-1.182527	1.219779
H	2.447768	-2.748962	0.890260
N	1.518078	-2.733151	-1.835859
H	2.468274	-2.836959	-2.225310
H	1.281523	-3.596818	-1.322452
H	0.866136	-2.658570	-2.630307
N	-2.522258	2.576176	-0.076048
H	-3.223835	2.721895	-0.819282
H	-2.466325	3.437041	0.490307
H	-2.874274	1.826074	0.536491
N	-0.615894	3.816418	-1.603039
H	0.226741	3.836346	-2.195646
H	-1.419662	4.066064	-2.200243
H	-0.505210	4.550151	-0.885127

(μ -OAc)₄ III-III

Mn	1.226918	-0.970315	-0.724068
O	2.528657	-0.056554	-1.764516
C	2.309153	1.175621	-2.126840
O	1.265425	1.815604	-1.815686
C	3.370522	1.811396	-2.978130
H	3.372645	2.899014	-2.844189
H	3.146466	1.595787	-4.035328
H	4.358460	1.392774	-2.754648
O	-1.395223	0.086100	0.264552
C	-1.203898	-1.109405	0.624658
O	-0.136985	-1.789860	0.312950
C	-2.212587	-1.822785	1.478302
H	-1.952370	-1.659640	2.536651
H	-2.192363	-2.902758	1.292481
H	-3.217310	-1.420356	1.306946
O	0.197582	2.434544	0.786198
C	1.111230	1.673586	1.319676
O	1.451943	0.556319	0.838835
C	1.777747	2.212567	2.552710
H	2.162421	1.395578	3.173260
H	1.090029	2.843461	3.127688
H	2.628592	2.841097	2.243860
O	-0.233221	-0.667094	-2.335507
C	-1.122124	0.055714	-2.867694
O	-1.494926	1.206833	-2.383772
C	-1.798503	-0.372126	-4.138450
H	-2.821281	0.018770	-4.189978
H	-1.797722	-1.464088	-4.228564
H	-1.238185	0.044894	-4.990772
Mn	-0.679697	1.867842	-0.800675

N	2.805518	-1.826092	0.586230
H	3.711098	-1.966395	0.127079
H	2.943506	-1.128584	1.324841
H	2.546446	-2.706497	1.042736
N	1.460795	-2.804665	-1.957259
H	2.390733	-2.924178	-2.371455
H	1.219722	-3.675326	-1.473053
H	0.795860	-2.691623	-2.729453
N	-2.646142	2.523452	0.004913
H	-3.352807	2.707922	-0.714376
H	-2.610359	3.339201	0.624411
H	-2.981022	1.731111	0.562782
N	-0.526559	3.903797	-1.677496
H	0.346451	3.899314	-2.214960
H	-1.281839	4.153698	-2.323718
H	-0.450440	4.652227	-0.981133

(μ-O)(μ-OH)	IV-IV		
O	1.110375	0.010702	1.494131
Mn	0.008206	-0.015273	3.001922
O	-1.226423	-0.037699	1.417165
Mn	0.115373	-0.005906	-0.079889
N	0.064034	-2.107788	3.288550
N	-1.512764	-0.060078	4.531835
N	-0.033216	2.077469	3.294476
N	1.660120	0.035319	4.308551
N	-1.324136	-0.031326	-1.696012
N	1.858120	0.022274	-1.258868
N	0.187154	-2.096014	-0.399483
N	0.090465	2.084486	-0.392558
H	0.171028	2.347141	-1.391956
H	-0.782242	2.538716	-0.076680
H	0.867901	2.580288	0.072600
H	0.284832	-2.352887	-1.398683
H	0.984572	-2.557736	0.066638
H	-0.665519	-2.589747	-0.088214
H	1.728148	-0.148231	-2.273448
H	2.376791	0.915878	-1.194731
H	2.536433	-0.689735	-0.934387
H	-1.922096	-0.876141	-1.720475
H	-2.001796	0.751077	-1.668439
H	-0.918354	0.019702	-2.648820
H	-0.000648	-2.394365	4.282152
H	-0.717133	-2.603869	2.829865
H	0.937643	-2.539299	2.944796
H	-0.116612	2.360772	4.287474
H	0.821410	2.550736	2.958047

H	-0.834158	2.536453	2.831397
H	1.857158	-0.846806	4.813608
H	2.512906	0.230182	3.752271
H	1.631280	0.757669	5.050597
H	-1.148600	-0.087525	5.502548
H	-2.153366	0.753398	4.521104
H	-2.147467	-0.876192	4.473108
H	-2.209141	-0.065348	1.385266

(μ-OH)₂	IV-IV		
O	1.247533	0.039497	1.496932
Mn	0.039801	0.015179	3.179745
O	-1.047726	-0.015198	1.419991
Mn	0.160733	0.004206	-0.262743
N	0.088454	-2.095505	3.521301
N	-1.604480	-0.025058	4.535577
N	-0.031267	2.128319	3.502282
N	1.589142	0.066999	4.644228
N	-1.387269	-0.034843	-1.728391
N	1.806173	0.034391	-1.617858
N	0.217928	-2.108679	-0.585124
N	0.125960	2.115076	-0.602419
H	0.153856	2.387202	-1.606832
H	-0.725922	2.577447	-0.233927
H	0.929970	2.613680	-0.177887
H	0.258374	-2.386980	-1.587426
H	1.042261	-2.569390	-0.156756
H	-0.613467	-2.604730	-0.213607
H	1.533979	0.022395	-2.624123
H	2.409356	0.875680	-1.512589
H	2.447068	-0.777256	-1.503100
H	-1.996519	-0.875555	-1.659864
H	-2.034618	0.777165	-1.662908
H	-1.046795	-0.028829	-2.713695
H	0.063574	-2.365516	4.526342
H	-0.712988	-2.600212	3.099077
H	0.942696	-2.553235	3.152522
H	-0.071950	2.407232	4.504382
H	0.795539	2.630364	3.128663
H	-0.860020	2.581800	3.074704
H	2.237227	-0.744932	4.585696
H	2.197451	0.907705	4.567808
H	1.248682	0.069101	5.629520
H	-1.332410	-0.010779	5.541879
H	-2.250118	0.782705	4.420212
H	-2.202937	-0.869891	4.431364
H	-2.034084	-0.045980	1.386017

H 2.234200 0.057814 1.530676

(μ-O)₂(μ-OH)	IV-IV		
O	1.129001	-0.113212	1.295481
Mn	0.020068	-0.074980	2.763074
O	-0.326952	-1.805477	2.277441
Mn	-0.091468	-1.264286	0.543524
O	-1.352981	0.147483	1.282564
N	1.486166	-0.604872	4.118307
N	-1.520835	-0.137013	4.206939
N	0.359195	1.999174	3.088702
N	-1.735164	-2.434835	-0.082442
N	1.287282	-2.743476	0.122095
N	0.133654	-0.399746	-1.386386
H	-1.769041	-2.794665	-1.046029
H	-1.848535	-3.249670	0.537283
H	-2.588415	-1.871894	0.046643
H	0.890485	0.298634	-1.352022
H	0.384368	-1.042607	-2.150778
H	-0.700799	0.101136	-1.723964
H	1.159116	-3.277324	-0.748987
H	2.235601	-2.341691	0.090063
H	1.286640	-3.431631	0.888493
H	0.699877	2.267099	4.022805
H	1.077813	2.326985	2.427028
H	-0.467828	2.591866	2.927747
H	1.448542	-0.171413	5.051514
H	1.452410	-1.623355	4.268169
H	2.417282	-0.396897	3.729028
H	-1.467989	0.467694	5.037974
H	-2.403906	0.099697	3.731799
H	-1.645741	-1.098939	4.553297
H	-1.307818	1.009781	0.818108

(μ-O)(μ-OH)₂	IV-IV		
O	1.310656	-0.039816	1.244967
Mn	0.059637	-0.061246	2.829551
O	-0.176820	-1.781869	2.252726
Mn	-0.058658	-1.315938	0.487430
O	-1.132196	0.180689	1.250370
N	1.414408	-0.575781	4.311498
N	-1.523853	-0.153323	4.155977
N	0.341965	2.010326	3.184884
N	-1.736394	-2.401257	-0.041412
N	1.195201	-2.890135	-0.006893
N	0.108765	-0.474199	-1.451696
H	-1.788160	-2.748835	-1.013816

H	-1.851837	-3.223994	0.575441
H	-2.578769	-1.818240	0.101819
H	0.818234	0.278166	-1.459945
H	0.396894	-1.119437	-2.206568
H	-0.760145	-0.036920	-1.803428
H	0.856919	-3.493221	-0.776408
H	2.145635	-2.596158	-0.291355
H	1.315599	-3.517553	0.806644
H	0.717240	2.267558	4.113414
H	1.015639	2.405537	2.507075
H	-0.515156	2.580786	3.085591
H	1.162541	-0.256993	5.262923
H	1.497479	-1.604872	4.375167
H	2.370823	-0.215584	4.149774
H	-1.483940	0.464350	4.984183
H	-2.399065	0.086205	3.659364
H	-1.652240	-1.117333	4.509416
H	-1.165040	1.048654	0.787343
H	2.257783	-0.290308	1.331854

(μ -OH) ₃	IV-IV		
O	1.268366	-0.237534	1.347988
Mn	0.037449	-0.044742	2.919750
O	-0.177278	-1.950037	2.334174
Mn	-0.086551	-1.383309	0.412546
O	-1.162941	0.046400	1.316738
N	1.417876	-0.482140	4.420219
N	-1.523411	0.006202	4.302029
N	0.369686	2.001909	3.143574
N	-1.751296	-2.435244	-0.273276
N	1.190245	-2.928074	-0.162443
N	0.144413	-0.440377	-1.432913
H	-1.798644	-2.564244	-1.304054
H	-1.835265	-3.393287	0.122870
H	-2.627664	-1.939585	-0.015492
H	0.889970	0.282038	-1.383176
H	0.415800	-1.065600	-2.218261
H	-0.710921	0.051208	-1.762294
H	0.828516	-3.541779	-0.919980
H	2.118446	-2.601282	-0.499280
H	1.382061	-3.561084	0.639309
H	0.727546	2.292861	4.075540
H	1.077345	2.333831	2.458557
H	-0.478214	2.583254	2.985990
H	1.142516	-0.180246	5.376433
H	1.572054	-1.507822	4.486817
H	2.355301	-0.059949	4.262896

H	-1.482330	0.787655	4.986804
H	-2.437321	0.109413	3.817989
H	-1.599207	-0.855709	4.879159
H	-1.449506	0.887163	0.881904
H	2.229550	-0.459400	1.418721
H	-0.852918	-2.572912	2.699693

(μ-OH)(μ-OAc)		IV-IV	
Mn	0.612469	2.443496	-0.057842
Mn	0.937501	2.515329	4.015870
O	0.556414	3.202316	1.980382
O	1.178362	0.860942	0.830007
O	1.347920	0.898830	3.106737
C	1.450999	0.273226	1.964117
C	1.881879	-1.141395	1.956047
H	2.531356	-1.383254	2.817374
H	0.980978	-1.799042	2.052902
H	2.367985	-1.423912	1.004728
N	-0.034449	4.249311	-0.982304
H	0.629024	5.042701	-0.898413
H	-0.192519	4.161596	-2.006034
H	-0.936199	4.616196	-0.623252
N	0.793351	1.399517	-1.910617
H	0.753271	1.977959	-2.773045
H	1.695374	0.887196	-1.945439
H	0.067072	0.667463	-2.027747
N	0.482437	4.364953	4.966392
H	0.696045	4.375313	5.983765
H	-0.514937	4.646916	4.916139
H	1.008577	5.178597	4.595026
N	1.365905	1.527467	5.857438
H	1.020929	1.991788	6.720803
H	2.381720	1.376294	6.006669
H	0.951843	0.575482	5.851927
N	2.590993	3.081913	-0.496407
H	2.741179	3.380205	-1.479903
H	3.289165	2.333107	-0.337252
H	2.903754	3.888986	0.069216
N	-1.422628	1.848508	-0.149411
H	-1.878283	2.007694	-1.069236
H	-1.543252	0.836453	0.037950
H	-2.031530	2.338292	0.527397
N	-1.061564	1.944827	4.450904
H	-1.352611	2.102459	5.435347
H	-1.226426	0.935429	4.285799
H	-1.769707	2.446059	3.888382
N	2.962257	3.146009	4.102195

H	3.194368	3.891596	3.424780
H	3.621987	2.370073	3.910237
H	3.258268	3.530691	5.020536
H	0.270567	4.142188	1.986539

(μ-OH)(μ-OAc)₂	IV-IV		
O	1.408323	2.870490	1.309454
Mn	0.961003	1.927326	3.041442
Mn	2.632004	2.126766	-0.117107
O	1.671343	0.482629	0.015862
O	0.604695	0.359361	2.012333
O	2.817106	1.520139	3.254295
O	3.880772	1.653492	1.253137
C	0.911998	-0.148935	0.858239
C	3.889588	1.414063	2.529417
C	5.158328	1.007524	3.176982
C	0.388622	-1.486464	0.496516
H	-0.564410	-1.702792	1.005646
H	0.290377	-1.604939	-0.594575
H	1.120722	-2.252514	0.840953
H	5.220536	-0.104695	3.150235
H	6.036375	1.390635	2.632844
H	5.188245	1.302762	4.238243
N	1.387218	2.629406	-1.743687
N	3.916887	1.165549	-1.455409
N	3.713232	3.914581	-0.430209
H	1.785372	3.265705	-2.456380
H	1.106954	1.774392	-2.255752
H	0.501020	3.071640	-1.448526
H	3.163543	4.790691	-0.401172
H	4.451434	4.013948	0.287286
H	4.215934	3.954835	-1.334682
H	3.608558	0.182585	-1.559753
H	3.993428	1.549245	-2.413911
H	4.876602	1.131798	-1.067725
N	-1.106785	2.334842	2.976383
H	-1.502622	2.863958	3.773124
H	-1.386536	2.862973	2.133220
H	-1.642176	1.449793	2.933054
N	1.225276	3.617898	4.280488
H	0.877721	4.517236	3.904974
H	2.229605	3.758939	4.482768
H	0.777495	3.536083	5.210686
N	0.631952	0.773601	4.752585
H	1.494545	0.726707	5.323739
H	0.421256	-0.197107	4.460206
H	-0.134097	1.057957	5.388312

H 1.205250 3.828707 1.262301

	(μ-O)(μ-OH)(μ-OAc)	IV-IV	
N	-3.650147	1.411324	2.720346
Mn	-2.706130	-0.035431	3.967426
N	-4.490352	-0.155786	5.061768
O	-1.217899	0.096228	2.761950
C	0.050961	0.099013	3.024512
O	0.474307	0.088969	4.249156
Mn	-0.531785	-0.040668	5.878843
O	-1.801530	-1.128688	5.128096
C	1.029147	0.116879	1.910544
O	-1.883548	1.264647	5.227345
N	-3.350183	-1.614949	2.786725
H	1.972966	0.590991	2.215770
H	1.259585	-0.932782	1.634189
H	0.609429	0.605669	1.019511
N	0.711519	-1.627245	6.368286
N	0.832837	1.400445	6.652409
N	-1.388269	-0.156467	7.788910
H	-4.365315	-1.715470	2.629383
H	-2.911433	-1.555778	1.853250
H	-3.031552	-2.504804	3.203572
H	-3.981193	2.258911	3.208799
H	-2.982049	1.739391	2.004661
H	-4.468303	1.078406	2.185323
H	-4.548881	-1.035812	5.596889
H	-4.551924	0.611316	5.748621
H	-5.363869	-0.101026	4.514474
H	0.990322	-1.733245	7.356394
H	0.253681	-2.513273	6.098989
H	1.585138	-1.571452	5.819545
H	-0.733483	-0.100070	8.584900
H	-2.061228	0.611240	7.936235
H	-1.911998	-1.035909	7.917565
H	1.454052	1.728541	5.895732
H	0.395469	2.248133	7.048214
H	1.471132	1.063189	7.390856
H	-1.646619	2.179282	4.959671

	(μ-OH)₂(μ-OAc)	IV-IV	
N	-3.627798	1.462978	2.716730
Mn	-2.817373	-0.056588	3.902910
N	-4.639025	-0.136118	4.962212
O	-1.258072	0.015154	2.799869
C	0.020625	0.033230	3.056362
O	0.439005	0.011128	4.291246

Mn	-0.454875	-0.063175	5.980212
O	-1.870954	-1.250054	5.205134
C	0.994539	0.070359	1.948563
O	-1.926206	1.098980	5.275853
N	-3.552909	-1.533085	2.618013
H	1.943700	0.543006	2.255846
H	1.239057	-0.977924	1.652396
H	0.574807	0.561942	1.053381
N	0.908452	-1.544431	6.545340
N	0.831377	1.450824	6.633733
N	-1.272426	-0.140610	7.922778
H	-4.450770	-1.308956	2.149468
H	-2.872606	-1.696562	1.852357
H	-3.714043	-2.451549	3.073076
H	-3.769913	2.360450	3.217671
H	-2.986467	1.665386	1.926899
H	-4.547714	1.253724	2.285752
H	-4.691114	-0.972619	5.569911
H	-4.753123	0.679080	5.590348
H	-5.504903	-0.161762	4.393197
H	1.450297	-1.348658	7.407811
H	0.479541	-2.474883	6.709184
H	1.612691	-1.672325	5.794512
H	-0.598261	-0.135681	8.709948
H	-1.903568	0.659965	8.103417
H	-1.845175	-0.991569	8.063618
H	1.505035	1.682628	5.879852
H	0.351909	2.336238	6.884318
H	1.409096	1.219377	7.463511
H	-1.814514	2.069875	5.152216
H	-1.719766	-2.207317	5.028941