

Supporting Information

How Bonding in Manganous Phosphates Affects their Mn(II)-³¹P Hyperfine Interactions

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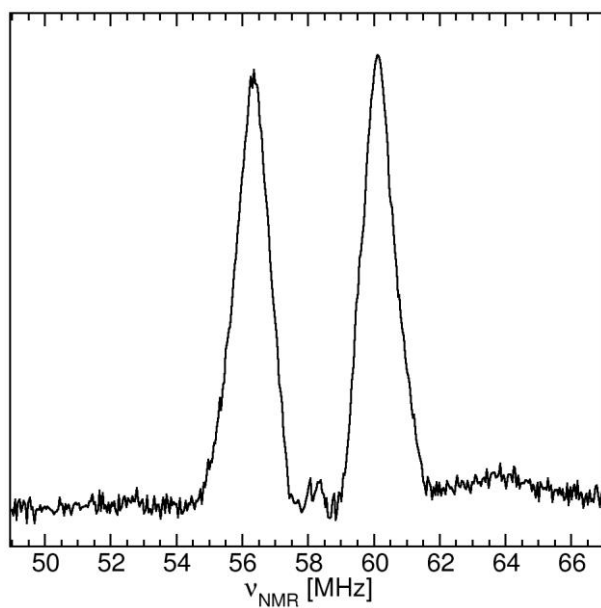


Figure S1. Typical raw 6 K Davies ^{31}P ENDOR spectrum of Mn(II) in orthophosphate solution. The particular spectrum was obtained at pH 11.

The atomic coordinates of the optimized geometries of the complexes in Table 1.

Mn (H ₂ O) ₅ (H ₂ PO ₄)			
O	-0.889674365462	0.910103496985	-0.149464516657
P	0.505506667449	0.301750645694	-0.015216086154
O	0.595017473572	-0.884912118252	-1.114001907106
Mn	-1.683713226108	2.418021954180	1.081859906438
O	-0.544435582094	1.542117367327	2.816394922588
O	0.116112293228	3.703763757880	0.579221254543
O	-2.338425979583	4.094971112542	2.365903400114
O	-3.377465616077	1.441414097763	2.203908921713
O	-3.274384607195	2.430182501460	-0.518092245113
O	1.487886878512	1.493743331750	-0.592187005840
O	0.977914720307	-0.155033112559	1.347198412411
H	2.427771482895	1.336438477940	-0.408133672462
H	0.005745492456	4.549925115906	0.122301433256
H	-0.074968171635	2.138792110400	3.415849264104
H	-3.207492868457	3.982713916009	2.779232278973
H	-3.710626512987	3.240629925501	-0.818754964774
H	-3.113395733818	0.796354924179	2.876527258367
H	-2.251791196590	5.032716900032	2.141933294112
H	0.112863586564	0.878845290553	2.478409967133
H	0.751559198639	3.178544280870	0.051896951684
H	-2.956659419672	1.974014936972	-1.312153455093
H	-4.088783718064	1.037121845741	1.686031863620
H	1.239837204120	-1.568277758872	-0.873553275856

Mn (H ₂ O) ₅ (NaPO ₄) ₂			
O	-0.067213740659	0.987385092446	1.840488892987
Mn	1.267057133473	2.449030112330	2.462945352765
O	0.235389973822	4.135829991134	1.184515134084
P	0.359203880258	-0.448449983104	1.322021735717
O	1.172066655295	-1.153655538466	2.472011900108
O	-0.870127818563	-1.286243554092	0.867446092897
O	1.291041629203	-0.243193933594	0.044834239796
O	2.319785364344	0.761655660501	3.670011509153
O	2.626062956275	1.833286382378	0.630736299299
O	2.593921732135	3.898592495211	3.128646104582
P	2.179224245145	5.376569769482	3.521530266540
O	3.393586462838	6.197480121274	4.042369511619
O	-0.082364809893	3.093178576386	4.256845957561
O	1.125662539720	5.277988363402	4.713855585567
O	1.505540714394	6.041464418117	2.262590818852
Na	-0.142029358474	-1.413658742026	-1.322901046469
H	2.658292485624	2.466473470820	-0.097778694606
H	3.274738353944	0.730660449145	3.528434095199
H	0.741207351241	4.971866043494	1.549431730597
H	0.337484182719	4.012213758818	4.499120390117
H	1.908903255421	-0.080932177493	3.213392669079
H	2.118821733844	0.990801720118	0.295820072209
H	0.393221447106	4.088230180147	0.232943291403
H	-1.002626671711	3.252131920018	4.010195993411
Na	2.445243302498	6.530315403554	6.128747097532

Mn (H₂O)₄ (PO₄)₂

O	-0.117724339773	1.092969035184	1.772147664415
P	0.075521080328	-0.440347345933	1.386664405132
O	-1.374638438307	-1.061850361714	1.212512376018
Mn	-1.135677096984	2.478497254833	0.606493307040
O	0.377830438049	4.165323143829	1.131606644993
O	-2.494064830300	3.282701740707	2.380648733951
O	0.097803819058	1.628415548668	-1.173624765033
O	-2.741211544152	0.777616657205	0.196146893195
O	-2.060396274647	3.889400816655	-0.606409157789
P	-2.395017412998	5.380430351535	-0.157074275231
O	-3.331645706924	5.281769158810	1.120421803747
O	0.821217496668	-0.470366013584	-0.015419882758
O	0.883939152998	-1.195215222793	2.468943434789
O	-3.080539778431	6.171482691142	-1.296767432141
O	-1.018622756345	6.052566407487	0.263810603897
H	-3.577130793784	0.889172556385	0.666265195001
H	-0.446791096104	1.424335999840	-1.944610843886
H	-2.908610947347	4.127424500280	1.897417602813
H	-0.171324744694	5.012059523041	0.807714671158
H	0.417917133047	0.710299801338	-0.753779865134
H	-2.231448790832	-0.038557780526	0.635669202817
H	-3.222889186353	2.698858544079	2.626058163495
H	0.520403617828	4.254940993533	2.082562519511

Mn	(H ₂ O) ₄ (HPO ₄) (PO ₄)		
O	-0.130945387977	1.088434373203	1.784393403330
Mn	0.082946092894	-0.893950018704	1.267476057093
O	-2.242640666142	-1.237833736265	1.094084252800
P	0.650671530865	1.730146133134	3.017316321699
O	2.199309294560	1.539556166896	2.724969269420
O	0.280348935051	3.215763327597	3.208341657239
O	0.264334106293	0.869880987923	4.298542496447
O	2.332840641715	-0.539899537854	1.350264082118
O	0.084191926598	-1.456062795951	3.473805134714
O	0.314019697419	-2.860373556562	0.529634598180
P	-0.606897036869	-3.726234130182	-0.374459476597
O	-0.133765754139	-5.156320579737	-0.600788033479
O	-0.057035255430	-0.308550708137	-1.044572096319
O	-0.427213919646	-2.893096641362	-1.859282503602
O	-2.105301000856	-3.572582185481	-0.009437337810
H	-0.707773648720	-1.895968248858	3.808406364177
H	2.837078510507	-1.225997859615	1.806261716621
H	-2.296484185110	-2.174229560680	0.698889490192
H	-0.261630021669	-1.163953920116	-1.490802042779
H	2.356683809428	0.338974727841	1.953996442625
H	0.134529486563	-0.465610967218	3.908919838530
H	-2.727439172621	-1.245622137155	1.929491904207
H	-0.800115525095	0.283348523860	-1.222068856771
H	-1.072818457619	-3.203247656577	-2.510730682034

Mn	(H ₂ O) ₄ 2 (HPO ₄)		
O	-0.182743448904	1.062689436650	1.884333905629
P	-0.004542548782	-0.405208800357	1.394101640822
O	-1.298329767550	-1.157968386384	1.125179940392
Mn	1.277354747811	2.430442648625	2.468371789538

O	2.373382908978	0.687753978910	3.432048262286
O	2.391040315002	1.955602131446	0.464810537861
O	2.733927663605	3.799419544858	3.051454845161
P	2.586524267650	5.308278474491	3.410236331732
O	1.718897654628	5.171555065128	4.877128211598
O	0.171360013711	2.969130542713	4.441921631736
O	0.111759861274	4.174055263825	1.523727111802
O	0.739807842950	-0.117814974440	-0.119650593141
O	1.056098301429	-1.166575496660	2.229052460814
O	1.626738860051	6.042994930585	2.440728293906
O	3.890457258959	6.028155218953	3.718287468512
H	1.053593200989	-0.944628311332	-0.514463524991
H	2.463781655873	2.657617761129	-0.195561750594
H	3.323563732908	0.643199526497	3.262492965468
H	0.660141169395	4.990860152335	1.795680444204
H	0.602148873154	3.810225019491	4.729837222717
H	1.938839613206	-0.122653209735	2.986281933860
H	1.865896469269	1.223584251148	0.058897889540
H	0.014211341161	4.184490872811	0.562870495080
H	-0.769400585561	3.162695453258	4.328616683986
H	1.420915598795	6.038207906052	5.189503802082

Mn (H₂O)₄ 2 (H₂PO₄)

O	-0.170273899767	1.048949397340	1.806460393558
Mn	1.276497763525	2.453349706681	2.436702461865
O	0.165095618610	4.179958516647	1.458170950067
P	0.093874241610	-0.382097475983	1.352133652470
O	0.991140401054	-1.269713653107	2.187511759478
O	-1.360015077879	-1.061729574185	1.110189853204
O	0.727996539829	-0.194145946629	-0.159700688690
O	2.407270610081	0.732741027661	3.372424626280
O	2.378332042547	2.050611183671	0.474557598077
O	2.712612912216	3.833221332333	3.142088766724
P	2.467805861000	5.299617876678	3.479762792049
O	3.919719643407	5.934100327112	3.830440737444
O	0.166664970389	2.861412880695	4.372800018391
O	1.675132445374	5.231526142458	4.926113079690
O	1.699410233707	6.168033929141	2.507480682753
H	1.121191613575	-1.009806624322	-0.508759986322
H	2.595197416771	2.775714900151	-0.127703671954
H	3.367034996628	0.707164993420	3.256151415422
H	0.627582897122	5.032968857448	1.658868038634
H	0.485632229564	3.684926526334	4.791800784235
H	2.044909075024	-0.125357065181	3.032839865200
H	1.923236837342	1.363007744589	-0.049780700868
H	-0.016851330225	4.157532245899	0.508900021797
H	-0.799629332927	2.906188285203	4.358818227211
H	1.271119516073	6.077443994947	5.176636607777
H	3.944002307106	6.896300095431	3.712669015159
H	-1.337380531756	-2.027363624430	1.195720700349

Mn (H₂O)₄ (H₃PO₄) (H₂PO₄)

O	-0.113832039190	0.954792496355	1.847026456362
P	-0.022588293393	-0.424844780451	1.276752234083

O	0.800162330682	-0.369201326793	-0.090969680136
Mn	1.315289686886	2.485429782170	2.379650765170
O	0.228780813282	2.773857462391	4.327214397572
O	0.148285903057	4.163347482076	1.463950351518
O	2.594808391054	0.873027348879	3.324653117311
O	2.372803396737	2.098093667881	0.420561838616
O	2.733291081938	3.853126559788	3.099684992295
P	2.445499824876	5.299452382818	3.495423098594
O	1.611486831574	6.160524482054	2.572373447668
O	0.820149876360	-1.479546394721	2.140182950942
O	-1.485856621742	-0.996549693310	1.041381734907
O	3.882193350384	5.975595163500	3.819849031667
O	1.704080731259	5.148956599918	4.960602808278
H	1.017878969879	-1.213218777627	-0.522226374098
H	2.629169007720	2.829733521275	-0.158666400352
H	3.539982515957	1.067825650472	3.403687578055
H	0.575986349911	5.026183487503	1.705534658385
H	0.539658561123	3.575467246375	4.792503450517
H	2.523452358584	-0.062325333039	3.079563586146
H	2.024258080232	1.392520250623	-0.149038146427
H	-0.034671763506	4.178229691569	0.514421126518
H	-0.738489935663	2.791559529377	4.346095133678
H	1.288692441451	5.972116778516	5.263473134022
H	3.871463298841	6.941075952788	3.729550957527
H	-1.556286491169	-1.914582212114	0.728722354601
H	0.384051342877	-1.802547018273	2.947641396580

Mn (H₂O)₄ 2 (H₃PO₄)

each phosphate donates a hydrogen-bond to a water ligand

O	0.843085	1.377633	-1.639841
Mn	-0.006653	-0.027759	0.097378
O	-0.944114	-1.827778	1.312884
O	-0.067461	-1.667564	-1.418955
O	-1.972147	0.460390	-0.474515
P	-3.380273	0.142280	-0.055084
O	-4.181168	-0.439242	-1.306946
O	1.995914	-0.515467	0.504759
P	3.379970	-0.095497	0.094231
O	4.294765	-1.390134	-0.036006
O	0.131360	1.919688	1.150344
O	-3.508265	-0.901187	1.134393
O	-4.094624	1.479272	0.432075
O	4.012798	0.859861	1.206653
O	3.456233	0.658041	-1.300751
H	0.664465	2.307640	-1.422892
H	0.482923	1.233838	-2.530040
H	-0.687642	2.380127	1.387049
H	0.747421	2.051891	1.886430
H	0.733758	-2.068788	-1.786735
H	-0.733031	-1.673029	-2.122865
H	-0.774744	-2.643966	0.813242
H	-0.615266	-1.983078	2.213296
H	-5.019954	1.405511	0.718200
H	-2.660223	-1.386943	1.303596
H	-5.013642	-0.899025	-1.107872

H	4.700304	1.474823	0.901654
H	5.247806	-1.243322	-0.154245
H	2.579194	1.038008	-1.567916

Mn (H₂O)₄ 2 (H₃PO₄)

each phosphate accepts a hydrogen-bond from a water ligand

O	-0.524710	0.416318	-2.062318
Mn	0.017393	-0.154741	0.030565
O	-2.016861	0.037246	0.629029
P	-3.418873	0.113061	0.111404
O	-4.186590	1.274613	0.882812
O	-0.044532	-2.322837	-0.497340
O	0.487016	-0.706314	2.136974
O	0.283680	2.011876	0.527533
O	2.083549	-0.240382	-0.498328
P	3.463254	-0.389854	0.054585
O	4.280493	0.959832	-0.150248
O	-4.289796	-1.219143	0.186510
O	-3.382014	0.413709	-1.457569
O	3.357503	-0.709081	1.623515
O	4.209770	-1.590940	-0.673840
H	-1.477926	0.442041	-2.254959
H	-0.863254	-2.741970	-0.800880
H	0.663092	-2.658526	-1.067408
H	-0.508660	2.559842	0.627983
H	0.911407	2.533880	0.006454
H	1.434776	-0.736294	2.354594
H	0.048699	-0.225993	2.854180
H	5.162198	-1.707284	-0.520395
H	4.168104	-0.925413	2.114095
H	5.173304	1.025476	0.227543
H	-4.470126	-1.557255	1.080244
H	-5.145707	1.336484	0.735763
H	-4.229973	0.438298	-1.932794

Mn (H₂O)₅ (methylo-PO₃)

2 water ligand hydrogen-bonds to 2 P-O

C	-0.070665662411	1.496872853801	0.953095762392
O	-0.258369837244	0.202603605610	0.361026586429
P	1.112892192522	-0.756470263768	0.060256904170
O	1.949888841046	0.031000887297	-0.980799723927
O	0.413470417866	-1.991398966640	-0.599537132585
Mn	-0.430542045211	-2.056925176461	-2.459185368089
O	-2.458742215755	-3.094895189697	-2.205593567111
O	1.793435180740	-1.034609128454	1.386958445750
O	0.265641651582	-4.191783727217	-2.801088875560
O	-1.841663873844	-0.381311663651	-1.744648464170
O	0.953910125538	-0.531669095887	-3.240455943013
O	-1.157443552381	-2.186685328333	-4.599825291014
H	1.624560822286	-0.807193172800	-3.880205859854
H	-2.032787061741	0.366768716443	-2.327163955439
H	-2.086153954578	-2.448886775223	-4.684553707422
H	0.452663212585	-4.473758329726	-3.708442474009
H	-3.034752730517	-2.526304936980	-1.672264543767
H	-1.020820303756	-1.441986810016	-5.202948624427

H	-1.370019803132	-0.019561366009	-0.949282782695
H	1.444804214481	-0.239115983147	-2.373702526007
H	1.018659871753	-4.479088655823	-2.264324282494
H	-2.497532023265	-3.980343571127	-1.816360658225
H	-1.059147075171	1.946414156580	1.069771406899
H	0.402298845456	1.401922827012	1.935650738019
H	0.546564763149	2.134266094216	0.310658936150

Mn (H₂O)₅ (methylo-PO₃)

1 water ligand hydrogen-bond to P-OCH3 and another to P-O

Mn	-0.426710820584	-2.046201459840	-2.473066471514
O	1.141331144532	-0.624580226691	-3.176604424228
O	0.200732262150	-4.176667817328	-2.927680300632
O	-1.202585225338	-2.118698128692	-4.594971373408
O	-2.462755648912	-3.047943676778	-2.182983193908
O	-1.726197573423	-0.394126832296	-1.588417082178
O	0.488268152551	-2.184991325016	-0.641588836577
P	1.006450703537	-0.876995210220	0.044917231088
O	-0.166917868619	0.047358681268	0.442080146423
O	2.087724041539	-0.182326458174	-0.815355306504
O	1.717218710547	-1.450749950107	1.417095530538
C	2.348153467072	-0.518784720960	2.307886972217
H	1.620972695100	0.197195329983	2.706119888725
H	2.767354246773	-1.101522183981	3.130555459186
H	3.153407772147	0.023557952931	1.800838427450
H	1.638919010503	-0.391436268702	-2.313876377747
H	1.791286071864	-0.943285117199	-3.817641709307
H	0.951459810336	-4.500546386483	-2.408757147519
H	0.371477886472	-4.428237886807	-3.846998823444
H	-1.057822981849	-1.384739507953	-5.209236542546
H	-2.143109531013	-2.345190421471	-4.647797088402
H	-2.511634252090	-3.945233872149	-1.823274367243
H	-2.985573975676	-2.478223006201	-1.598072128983
H	-1.920827102917	0.400587328957	-2.103467100065
H	-1.207853994701	-0.106100836093	-0.759264381424

Mn (H₂O)₅ ((methylo)₂-PO₂)₂

both conformation 1

O	-0.120352	1.030527	1.891067
P	0.217780	-0.406611	1.486425
O	0.787197	-0.270865	-0.040818
Mn	1.239831	2.560165	2.403045
O	0.109560	3.053085	4.348941
O	-0.056225	4.167852	1.481719
O	2.452270	0.967206	3.444014
O	2.278849	2.114659	0.414516
O	2.659248	4.031699	2.934733
P	2.317147	5.444139	3.431226
O	1.233677	6.177271	2.667643
O	1.181640	-1.158357	2.384562
O	-1.133945	-1.254644	1.212889
O	3.676226	6.306482	3.591981
O	1.832250	5.363053	4.989095
C	1.292481	-1.440462	-0.730744
H	2.443438	2.808341	-0.239022

H	3.413025	0.980851	3.336311
H	0.329429	5.033809	1.791622
H	0.421591	3.868788	4.783338
H	2.127781	0.075884	3.142448
H	1.835926	1.374877	-0.046940
H	-0.145232	4.212004	0.520087
H	-0.854435	3.121192	4.295399
C	2.736376	4.879821	6.015600
C	4.566385	6.467493	2.464712
C	-1.849296	-1.848165	2.319852
H	1.651767	-1.092320	-1.699050
H	2.112536	-1.889550	-0.165551
H	0.488752	-2.166926	-0.872271
H	-2.668934	-2.417367	1.881237
H	-1.193210	-2.514461	2.885092
H	-2.251941	-1.071538	2.976513
H	5.410494	7.055044	2.825666
H	4.914810	5.493245	2.112468
H	4.065207	7.003789	1.653914
H	2.149931	4.820039	6.932452
H	3.120355	3.890390	5.753445
H	3.562017	5.582312	6.144021

Mn (H₂O)₅ ((methylo)₂-PO₂)₂
conformation 1 and 2

C	1.139800373495	-1.362586126698	-0.893691537750
O	0.678227752840	-0.232481578848	-0.113565929152
P	0.199288987229	-0.447647203680	1.435166128044
O	-1.165732088294	-1.284835930971	1.197235997964
C	-1.818559487811	-1.934898573137	2.311002213278
O	-0.115503673331	0.966132298236	1.930937209246
Mn	1.271731237459	2.466006778229	2.453261266591
O	2.667808467507	3.966176607816	2.907094044879
P	2.609151001901	5.337461024979	3.580361886950
O	1.789315915607	5.152683791001	5.005341727534
C	2.475033346039	5.287870240730	6.273369544902
O	1.213962173816	-1.239567198033	2.237461982761
O	0.307132051308	2.857382116799	4.466029706155
O	-0.096970475383	4.102302872742	1.638759107098
O	2.558117660397	0.827718180340	3.326622928516
O	2.184845749691	2.138062743537	0.374318614040
O	1.469531405931	6.136418561318	2.707218997605
O	3.860969321235	6.136071085451	3.779019142761
H	2.290590212340	2.872876187452	-0.245660380246
H	3.508130834113	0.843538531009	3.146978126016
H	0.324942936019	4.964522917335	1.841059649459
H	0.684514169191	3.685296614997	4.835954003347
H	2.206858998943	-0.044411085392	2.999433524629
H	1.716809088499	1.421022565398	-0.097979331510
H	-0.326763161693	4.108334536552	0.699305185317
H	-0.655618639597	2.946958744173	4.496835386901
H	1.452461779543	-0.961097315783	-1.857525787198
H	1.984070058780	-1.846751929866	-0.397277340202
H	0.324544599307	-2.076076556898	-1.035697106603
H	-2.668540957340	-2.473453222928	1.891822164945

H	-1.136284108319	-2.636207173965	2.797465816407
H	-2.173799648935	-1.194163185945	3.033237059748
H	1.699320499430	5.286891578825	7.039692288622
H	3.154056534479	4.445762528744	6.433077284057
H	3.031862784794	6.225638502694	6.302394706376
C	1.132333710288	7.504124027991	3.037286032237
H	0.396146947522	7.825737849070	2.300526620875
H	0.701159319670	7.555295194302	4.040643807219
H	2.021396323329	8.135638002426	2.975611258182

Mn (H₂O)₅ ((methylo)₂-PO₂)₂

both conformation 2

C	4.725492515994	-1.621162289422	-1.002345493586
O	3.438521005306	-1.262990352986	-0.449473812497
P	3.289975038301	-0.035743892033	0.641440553405
O	3.404783238195	1.319018906349	-0.292997078921
O	4.374353038861	-0.076323417840	1.674143813902
C	4.631701701689	2.078501064218	-0.397228183051
O	1.815788026008	-0.103414656372	1.031599453588
Mn	-0.024269301547	-0.051263141614	0.023171293102
O	0.896364174741	-1.414827177091	-1.542631704074
O	-1.849659776858	0.025574492631	-1.012819728445
P	-3.325224740783	-0.017936158267	-0.614051668016
O	-4.391489948522	0.062854449866	-1.663485542981
O	-0.963764379609	1.285946407537	1.594939124393
O	-0.844094312447	-1.819867893224	1.204393792205
O	0.779284049669	1.744662227521	-1.100879873328
O	-3.556968227085	1.125025962079	0.559245014493
C	-4.262710213729	2.351561351915	0.252578222298
O	-3.431757774056	-1.373961277248	0.306387466592
C	-4.705583641213	-1.768673416299	0.868454292500
H	0.489176550735	-2.267577321360	-1.748246846231
H	0.609135591877	1.803586459203	-2.051257676702
H	-1.791826065384	-1.913974157031	0.969061215358
H	-1.930377445452	1.342550985675	1.433402103490
H	1.752127174382	1.783854018879	-0.978046221007
H	1.830279440140	-1.585647702921	-1.293317885277
H	-0.436848542351	-2.692681774081	1.115894318304
H	-0.844711152429	1.054670374142	2.526670974235
H	4.604713875368	-2.605207080450	-1.456120976817
H	5.023302895535	-0.899218478096	-1.767887920806
H	5.477208489794	-1.665869100839	-0.211478148849
H	4.368022362039	3.017141373872	-0.885402137106
H	5.041771744977	2.272890125071	0.595214769682
H	5.364575033966	1.542071795527	-1.004940430891
H	-4.405338036928	2.866306649037	1.203142214434
H	-3.669672656481	2.976464405584	-0.421170683567
H	-5.228537639912	2.125778609152	-0.202206246729
H	-4.532977949761	-2.710577630301	1.389251833536
H	-5.056760317185	-1.011727856613	1.574652673537
H	-5.439279122669	-1.911908179945	0.072159798729

Mn (H₂O)₅ (K(methylo)₂-PO₂)₂

Both Configuration-2

C	4.766626439430	-1.666292502584	-0.768419175657
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O	3.462835517785	-1.286394499583	-0.269066847352
P	3.278807164076	-0.006446750518	0.745035333883
O	1.793973423716	-0.040519810037	1.086778337710
Mn	-0.013056125283	-0.021702766207	0.016192687451
O	0.853193633603	1.710255812173	-1.154192614448
O	3.457185010286	1.297926211965	-0.239931277031
C	4.684146233754	2.065152289679	-0.298656827502
O	4.319181227744	-0.006007110482	1.827066561178
O	0.944616994218	-1.471851855261	-1.447590200898
O	-1.804408405537	0.079277377734	-1.077568921042
P	-3.290847504451	0.019510589950	-0.736847458071
O	-3.441732636895	-1.386334156775	0.090991273125
C	-4.739741177642	-1.804019569060	0.578723385835
O	-0.979559177836	1.373383373952	1.513471636234
O	-0.911410099671	-1.746881720245	1.206031342077
O	-4.314371799696	0.157705685742	-1.826102728528
O	-3.572340325951	1.103633030321	0.472431188307
C	-4.382951810011	2.283651412798	0.248118452055
H	0.531367796082	-2.322224428284	-1.651049872441
H	0.710495201205	1.740573654104	-2.110442542982
H	-1.833843203872	-1.877607028874	0.900899135528
H	-1.947159801902	1.398076503773	1.354854045874
H	1.821425699157	1.750349120331	-1.005121439998
H	1.865333804704	-1.651696716040	-1.162547672847
H	-0.480860019836	-2.613021440484	1.199620330045
H	-0.850365911619	1.201513922835	2.456698546054
H	4.647502117310	-2.650502206142	-1.221612083487
H	5.105235121974	-0.953261575333	-1.524918703344
H	5.484927939855	-1.719244793683	0.052448748817
H	4.436003011202	2.996559404882	-0.807885546689
H	5.048778997139	2.272071789918	0.708598274486
H	5.443724115056	1.524497620445	-0.868238098151
H	-4.561328423548	2.718710211415	1.231717746935
H	-3.848530572930	2.999058674527	-0.382648139529
H	-5.329636072166	2.008152099375	-0.218666030470
H	-4.591728009818	-2.775497617064	1.049895422734
H	-5.114983931839	-1.086540746618	1.313007265131
H	-5.440809106621	-1.895756088500	-0.253715179895
K	5.831856614305	-0.266220468611	3.955545575768
K	-5.815766945479	0.449473064466	-3.957559928865

Mn (H₂O)₄ (Methyl-OPO₃-PO₃)

C	-2.902379629206	-1.902104008007	-1.285597705194
O	-1.663740497257	-1.718463083179	-0.572095901765
P	-1.622221957400	-0.754985881648	0.778263276019
O	-1.937773091671	0.726953106160	0.201371678593
O	-0.154394215058	-0.862086310239	1.211649236644
Mn	1.489741041796	-0.201255424858	0.036847003640
O	2.974143937987	-1.752805518040	0.846495976307
O	-2.708762297079	-1.149359783772	1.739908486717
O	1.932812829467	1.427737530571	1.484868890290
O	1.011162932655	-2.080284835295	-1.255862135878
O	0.275765287637	1.045886232944	-1.093345982784
O	3.340013285668	0.283965176896	-1.186082290965
H	1.216162324052	-2.044463067891	-2.200574590153

H	4.044133309427	-0.380548232131	-1.189667935618
H	2.694724856187	1.984646855899	1.275034550370
H	2.669510304674	-2.632529370370	0.576645502927
H	3.255622554806	0.606856841715	-2.094640665687
H	0.030778816097	-2.101415677416	-1.182154142431
H	1.086636557081	1.987259181963	1.315460643100
H	3.169700931914	-1.808814821201	1.792928542815
H	-2.690549520850	-2.580569065776	-2.113130504702
H	-3.656547951812	-2.344243096453	-0.629169094320
H	-3.263441018283	-0.946306609404	-1.676843462036
P	-0.828038346108	1.899193051351	-0.388631215956
O	-1.666953704727	2.758336824778	-1.313274272878
O	-0.267554430523	2.588723226700	0.877670906045

Mn (H₂O)₄ (Methyl-OPO₃-PO₃-PO₃)
bidentate

Mn	1.780015615681	-0.250459109762	0.176654316883
O	1.527432954832	-2.419518433334	-0.562922654481
O	3.634787158870	-1.158380707667	1.148912444721
O	3.320747262516	0.179677479341	-1.441717011812
O	0.394251260358	-0.818156401866	1.679840602925
O	0.281455161901	0.551526670490	-1.014762612865
O	2.125633857440	1.707804286268	1.183996006342
P	-0.862203223220	1.382169278206	-0.347566120098
O	-1.705531201619	0.229723549927	0.607557062756
P	-1.109458335215	-1.021928727298	1.442144591005
O	-1.132460123860	-2.273247331265	0.351796650293
P	-2.354966574968	-3.314751911121	-0.110770036806
O	-1.553791802879	-3.753037652121	-1.489534990759
C	-2.083492257167	-4.846937978559	-2.253939531746
O	-2.414594116454	-4.483277890172	0.845724990351
O	-3.610295229845	-2.544338743043	-0.445736152871
O	-1.999067753948	-1.316165590171	2.616434793794
O	-1.918099653425	1.904370943575	-1.301506795871
O	-0.286967181634	2.399475113278	0.666465933314
H	3.941143667990	-0.801691631454	1.995244950394
H	3.566571117252	-2.117308677398	1.267774797438
H	3.017927687600	0.278480073518	-2.355748310007
H	4.127537689962	-0.354442989398	-1.471400382013
H	2.760041364579	2.305562491897	0.765817763103
H	1.187255962381	2.096507129397	1.023742400534
H	1.672836753619	-2.612720958012	-1.499484915849
H	0.577263623799	-2.591839825149	-0.388942777263
H	-3.094227842543	-4.623001396867	-2.612986225842
H	-2.101933364435	-5.766864479331	-1.660544865761
H	-1.420862477568	-4.981178581910	-3.110843919809

Mn (H₂O)₃ (Methyl-OPO₃-PO₃-PO₃)
tridentate

C	3.825266403725	1.149551866978	-4.361610757691
O	2.893263401229	1.830468521848	-3.502989277959
P	3.352150670532	2.179172515467	-1.966757192702
O	4.516269793102	3.132378759840	-1.943339241585
O	2.013164275957	2.989044921378	-1.491671302853
P	0.470884196098	2.455409379625	-1.137623116498

O	-0.479460279561	3.073128202056	-2.124352119535
O	0.538199477370	0.929523468158	-1.013090003113
Mn	2.093197763562	0.104265932957	0.243092042190
O	3.489958242650	0.863934144785	-1.185479529493
O	2.053839194013	1.747634241050	1.537423098338
P	0.704574920436	2.469161494143	1.843752415865
O	0.239118450115	3.123013060085	0.317553015981
O	2.424289519684	-1.858133969553	-0.948088932681
O	0.446351464435	-0.875021654878	1.444595886892
O	3.632968149022	-1.020043377696	1.531930897766
O	0.810798695268	3.692261432021	2.735089427753
O	-0.401334015273	1.449671601996	2.201700266595
H	4.068635870072	-1.735492102790	1.045804604720
H	4.335841406163	-0.514029681181	1.964052710972
H	0.753579816153	-1.381739584851	2.208490935952
H	1.678662262898	-2.439689900464	-1.155072619039
H	2.807827606378	-1.592956752585	-1.797646758622
H	3.329358483629	1.029573422986	-5.326038692365
H	4.079555758327	0.163699098183	-3.958774320834
H	4.737289509050	1.740695718176	-4.491967110051
H	0.031790964966	-0.013413757732	1.806909671996