Supporting Information for "Metavanadate at the active site of the phosphatase VHZ"

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Below are the absolute energies (in Hartrees) and the atomic coordinates of the structures that were computationally analyzed. The coordinates were obtained from the x-ray structure.

Complex shown in Figure 2A:

E(B3LYP/6-31G*) = -5421.28129098

C	-2.564078	6.097605	-2.147937
C	-2.074282	4.809721	-2.298077
C	-2.828828	3.841212	-2.936995
C	-4.073112	4.184683	-3.423734
C	-4.564762	5.465201	-3.268804
C	-3.806093	6.421611	-2.631369
C	-2.315088	2.454911	-3.101813
C	-3.178162	1.397957	-2.402183
C	-2.845657	0.007788	-2.952113
O	-3.652161	-0.583823	-3.667401
N	-3.103828	1.543927	-0.941127
C	-4.186200	1.758800	-0.201678
O	-5.342292	1.748475	-0.648949
C	-3.991763	2.009069	1.284148
N	-2.643245	2.312415	1.734752
C	-2.156038	3.555649	1.711129
O	-2.811871	4.525966	1.325986
C	-0.711852	3.757697	2.159414
C	0.139054	4.047198	0.919841
C	1.604621	4.421267	1.126244
C	1.817242	5.327482	2.313061
N	-0.168211	2.644116	2.945790
C	0.065405	2.731680	4.255662
O	-0.222864	3.729175	4.930432
C	0.702578	1.486602	4.903246
C	2.208904	1.429259	4.622323
N	0.038880	0.261248	4.467666
C	-1.157248	-0.032245	4.961671
O	-1.698806	0.657185	5.826250
C	-1.853628	-1.304514	4.472887
N	-3.291855	-1.056816	4.482188
C	-1.360245	-1.841526	3.108760

S	-1.835093	-0.855900	1.673917
V	0.198156	-0.347226	0.543004
O	0.639040	-1.848475	-0.195223
O	-0.408457	0.847159	-0.483213
O	1.124727	0.154276	1.848070
C	2.170170	5.052550	-0.139512
N	-1.666263	-0.511593	-2.655395
C	-1.184227	-1.724278	-3.297674
C	-1.768774	-2.997412	-2.727347
O	-2.611233	-3.650042	-3.354617
N	-1.342354	-3.346069	-1.520591
C	-1.856383	-4.536348	-0.860530
C	-3.360347	-4.421715	-0.633147
O	-4.108995	-5.362964	-0.917708
C	-1.090184	-4.757891	0.449855
C	0.388416	-5.150963	0.229796
C	1.215266	-5.066767	1.501703
N	1.551456	-3.683642	1.851085
C	2.250850	-3.333675	2.930953
N	2.518622	-2.051964	3.179963
N	-3.798787	-3.260691	-0.156681
C	-5.209695	-3.008286	0.089763
C	-6.025967	-3.105870	-1.196346
O	-5.655896	-2.518798	-2.199737
N	2.690387	-4.265005	3.773083
C	-5.405523	-1.614876	0.724107
O	-4.935639	-1.659815	2.073267
C	-6.865303	-1.197231	0.749411
O	-7.063408	-3.773521	-1.242127
N	2.912325	0.452939	-0.974720
C	3.663337	1.545394	-0.919259
N	3.545988	2.482147	-1.856543
N	4.546597	1.707043	0.060695
C	5.422844	2.869734	0.166581
C	6.387897	2.756612	1.330761
C	5.706988	3.008483	2.669403
O	1.942221	2.044727	-4.103413
C	1.503987	0.880095	-4.282680
O	1.615513	-0.025316	-3.430465
C	0.834520	0.551134	-5.594611
C	1.533546	-0.579303	-6.317362
O	5.363528	-0.578767	1.505494
C	4.959816	-1.690444	1.095837
O	3.993422	-1.819585	0.308681
C	5.710443	-2.922476	1.561836
C	5.098360	-4.224968	1.051585

C	6.216263	0.643233	-2.934691
C	5.598078	0.022967	-4.005037
C	5.633930	-1.358612	-4.119179
C	6.283716	-2.134160	-3.165843
C	6.888214	-1.500961	-2.090181
C	6.853870	-0.113721	-1.971079
C	6.302191	-3.623501	-3.287680
H	4.104848	-4.115862	1.069705
H	5.705043	-2.939110	2.561872
H	6.652879	-2.864288	1.233526
H	7.051832	-3.978678	-2.729838
H	6.457311	-3.861909	-4.245958
H	5.186899	-1.802454	-4.896487
H	5.126250	0.570192	-4.696387
H	6.201896	1.640568	-2.858431
H	7.289773	0.333493	-1.190166
H	7.353614	-2.046095	-1.393309
H	-3.643441	-0.240423	4.024463
H	-1.614621	-2.044477	5.102165
H	-0.361489	-1.884784	3.136593
H	-1.730929	-2.761978	2.987507
H	0.479126	-0.347375	3.807347
H	0.577042	1.562436	5.892545
H	2.638512	2.278941	4.929531
H	2.361494	1.314877	3.640217
H	2.611146	0.656060	5.113326
H	0.035401	1.783030	2.479621
H	-0.689231	4.534758	2.788130
H	0.119238	3.227482	0.348217
H	-0.294972	4.804410	0.431812
H	2.097503	3.573545	1.323611
H	3.129897	5.293020	0.007048
H	1.650798	5.877830	-0.361966
H	2.101692	4.401797	-0.895880
H	2.790171	5.539210	2.400579
H	1.500385	4.869409	3.143309
H	1.301839	6.174811	2.182856
H	-2.064508	1.569458	2.071884
H	-4.294251	1.188573	1.769831
H	-4.574509	2.780846	1.538133
H	-2.213194	1.479784	-0.490838
H	-4.146067	1.536835	-2.610536
H	-1.391624	2.412522	-2.721526
H	-2.283865	2.242885	-4.078364
H	-4.625643	3.496791	-3.894918
H	-5.471948	5.698254	-3.619004

H	-4.159995	7.350616	-2.521352
H	-2.011251	6.791787	-1.686771
H	-1.168424	4.578711	-1.942246
H	-1.091731	-0.060059	-1.973113
H	-1.417379	-1.679104	-4.269589
H	-0.190397	-1.761200	-3.194248
H	-0.657733	-2.782962	-1.057527
H	-1.714022	-5.334325	-1.445667
H	-1.118162	-3.911535	0.981588
H	-1.540473	-5.489146	0.961545
H	0.421523	-6.090689	-0.111435
H	0.785364	-4.534370	-0.450413
H	0.693399	-5.470835	2.253064
H	2.062903	-5.580716	1.369386
H	1.236286	-2.956607	1.241177
H	3.215010	-3.999812	4.582146
H	2.496436	-5.230006	3.596297
H	3.043513	-1.800004	3.992505
H	2.194125	-1.342341	2.554012
H	-3.136784	-2.537093	0.038861
H	-5.535402	-3.709472	0.723539
H	-4.898375	-0.953515	0.172399
H	-6.946564	-0.291886	1.166792
H	-7.392686	-1.858153	1.283460
H	-7.220029	-1.165572	-0.185109
H	-5.056209	-0.762827	2.498372
H	1.618130	-1.351587	-5.687042
H	2.445032	-0.265536	-6.585061
H	0.847665	1.364528	-6.177001
H	-0.111991	0.284000	-5.416235
H	5.229480	2.176840	2.954108
H	5.048045	3.753336	2.565536
H	7.118584	3.428507	1.210372
H	6.778580	1.835889	1.336898
H	4.860315	3.686151	0.293082
H	5.947913	2.954557	-0.679509
H	4.614491	0.996552	0.761104
H	2.883617	2.367963	-2.596805
H	4.120282	3.300496	-1.820645
H	2.249991	0.338708	-1.715007
H	3.008410	-0.256297	-0.276513
H	6.455486	3.281923	3.411631
H	5.403442	-5.046927	1.697518
H	5.442600	-4.414406	0.035941
H	5.354065	-4.028215	-2.936703
H	0.947721	-0.870826	-7.187849

H	-3.921634	-1.728595	4.072121
H	-3.778547	-0.946061	5.357932

Complex shown in Figure 2B:

E(B3LYP/6-31G*) = -4901.42875623

C	1.727809	-3.634447	0.694462
C	1.534656	-4.937697	1.214981
C	0.789643	-5.177939	2.374034
C	0.238858	-4.058681	2.966769
C	0.418934	-2.772195	2.447145
C	1.150954	-2.505815	1.300343
O	1.313912	-1.191292	0.823651
V	-0.178825	-0.082110	-0.199831
O	0.015483	-1.328264	-1.610982
S	-2.033199	1.040534	-1.380700
C	-1.580835	1.265999	-3.139307
C	-2.523536	0.665752	-4.191768
C	-2.444495	-0.853382	-4.300928
O	-3.332658	-1.451832	-4.889324
N	-3.916007	0.860783	-3.859496
N	-1.421330	-1.509442	-3.782888
C	-1.438805	-2.971294	-3.828894
C	-2.382298	-3.551682	-2.733723
O	-3.269642	-4.376542	-3.023285
C	-0.018669	-3.537010	-3.749231
O	-0.032582	-4.954399	-3.726518
N	-2.207915	-3.096254	-1.491983
C	-3.023011	-3.542385	-0.374403
C	-4.176822	-2.591690	-0.082012
O	-5.166811	-2.987161	0.536400
C	-2.175192	-3.706508	0.870188
N	-4.051352	-1.339991	-0.513731
C	-5.115785	-0.363870	-0.316466
C	-5.189436	0.276766	1.052562
O	-6.260771	0.730773	1.450842
N	-4.063602	0.316066	1.772424
C	-4.009606	0.924449	3.106474
C	-2.926851	1.995037	3.258521
O	-3.181200	3.058049	3.800787
C	-3.807687	-0.170324	4.171845

C	-5.075728	-0.993166	4.336565
C	-2.669698	-1.107453	3.763119
C	-2.385786	-2.198536	4.771378
N	-1.725030	1.718731	2.757149
C	-0.593441	2.611285	2.950550
C	-0.587122	3.913613	2.200356
O	-0.758003	4.989356	2.786739
N	-0.371502	3.818488	0.884910
C	-0.359712	4.989654	0.048258
C	-1.798885	5.451274	-0.083670
O	-2.078995	6.663586	-0.095901
C	0.266551	4.703487	-1.318377
C	1.740247	4.338870	-1.261433
C	2.198336	3.688475	-2.556632
N	1.849414	2.270835	-2.611525
C	2.355226	1.411695	-3.489091
N	1.977220	0.140861	-3.463878
N	-2.724702	4.501564	-0.182743
C	-4.139673	4.869363	-0.237593
N	3.236832	1.822744	-4.389483
O	-1.454465	-0.472374	1.160609
O	0.787256	1.523491	-0.015362
O	3.576364	-0.701956	-0.384177
C	4.157960	-1.433388	-1.207098
O	3.872275	-2.649856	-1.357554
C	5.237784	-0.789508	-2.049276
C	5.362564	0.714788	-1.785704
C	6.130834	0.988061	-0.491544
O	7.341321	0.818263	-0.438913
N	6.036255	1.386014	-2.880664
N	5.415129	1.440272	0.534521
C	5.998837	1.741698	1.850364
C	6.736438	0.524842	2.429018
C	5.822616	-0.498080	3.076973
C	5.221561	-1.484802	2.327408
C	4.383723	-2.419125	2.910239
C	4.148191	-2.380328	4.244300
C	4.764458	-1.420793	5.024519
C	5.592356	-0.480179	4.434102
H	5.018500	-0.929077	-3.014395
H	6.112356	-1.226017	-1.838695
H	4.432811	1.072626	-1.701020
H	5.541278	1.213516	-3.732450
H	6.970479	1.037538	-2.961593
H	4.433709	1.582367	0.405585
H	5.244703	1.962981	2.469019

H	7.234000	0.076320	1.686751
H	7.385253	0.848849	3.117842
H	5.394406	-1.526631	1.343459
H	3.951665	-3.122955	2.346899
H	3.529242	-3.045253	4.663222
H	4.613424	-1.405066	6.012781
H	6.027344	0.219745	4.999956
H	-4.101129	1.838264	-3.758141
H	-4.122666	0.392196	-3.001056
H	-2.229159	1.130634	-5.027187
H	-0.680034	0.853199	-3.272545
H	-1.525781	2.249642	-3.311284
H	-0.654331	-1.019008	-3.369770
H	-1.813222	-3.259208	-4.710505
H	0.499921	-3.228665	-4.546117
H	0.420141	-3.202036	-2.915675
H	0.905050	-5.296945	-3.674268
H	-1.488633	-2.422431	-1.323354
H	-3.412870	-4.425399	-0.637266
H	-2.751233	-4.013590	1.627892
H	-1.753884	-2.829963	1.105029
H	-1.460050	-4.384495	0.700287
H	-3.211877	-1.063271	-0.981607
H	-4.988591	0.365725	-0.987907
H	-5.987766	-0.824879	-0.484752
H	-3.230657	-0.082586	1.388945
H	-4.885642	1.389256	3.235763
H	-3.582558	0.280148	5.036399
H	-2.912463	-1.536753	2.893828
H	-1.838998	-0.562515	3.646415
H	-1.634547	-2.770261	4.441513
H	-3.203766	-2.760738	4.893921
H	-2.131140	-1.785952	5.646347
H	-4.928209	-1.698246	5.030770
H	-5.307427	-1.426487	3.465997
H	-5.826356	-0.397099	4.622366
H	-1.597189	0.876399	2.234315
H	-0.549340	2.829740	3.925307
H	0.228993	2.109908	2.683817
H	-0.216312	2.919681	0.474956
H	0.203953	5.706047	0.458214
H	-0.229242	3.942905	-1.737380
H	0.166730	5.520203	-1.886524
H	2.275584	5.168960	-1.106957
H	1.888861	3.700674	-0.505735
H	1.762803	4.158193	-3.325160

H	3.191574	3.778888	-2.629466
H	1.187679	1.925576	-1.945533
H	3.616833	1.174727	-5.049857
H	3.521633	2.780681	-4.408593
H	2.357268	-0.507184	-4.124196
H	1.311902	-0.169868	-2.784674
H	-2.455256	3.539183	-0.219361
H	-4.709168	4.054027	-0.342018
H	-4.423733	5.392402	0.565986
H	-4.262434	5.458260	-1.036423
H	0.603659	-6.068417	2.789313
H	-0.308115	-4.171757	3.796790
H	-0.002806	-2.003651	2.929052
H	2.288940	-3.515455	-0.124973
H	1.945159	-5.714058	0.736932
H	6.687273	2.582278	1.776871
H	6.062033	2.377705	-2.701919
H	-4.492953	0.484042	-4.595202

Complex shown in Figure 2C:

E(B3LYP/6-31G*) = -5203.76225829

C	-4.650931	-3.875018	3.942494
C	-5.278665	-4.241590	2.771297
C	-5.628832	-3.288152	1.825213
C	-5.322039	-1.959816	2.070362
C	-4.697310	-1.589556	3.237779
C	-4.359132	-2.550930	4.174980
C	-6.284062	-3.692621	0.544783
C	-5.305790	-3.787446	-0.629041
N	-5.017139	-2.467767	-1.186787
C	-5.973152	-1.657321	-1.629435
O	-7.177812	-1.931931	-1.565809
C	-5.500137	-0.338456	-2.237071
N	-6.163584	-0.116872	-3.514996
C	-5.767077	0.823982	-1.273457
C	-4.801517	0.836201	-0.084474
O	-3.860552	0.006070	-0.059148
O	-4.988004	1.679369	0.825546
N	-5.392620	4.285088	0.301963
C	-6.239458	5.176589	1.133674
O	-1.546300	-0.181465	1.461650
V	-0.002954	0.388743	0.152605
O	1.311197	-0.168568	1.419883

S	1.883731	1.195505	-1.300103
C	1.208610	2.388941	-2.470610
C	1.920465	3.745262	-2.495497
C	1.432286	4.689840	-1.404799
O	1.992607	5.762388	-1.233670
N	3.354112	3.612265	-2.305461
N	0.404434	4.319671	-0.657937
C	0.014065	5.166578	0.458862
C	0.902312	4.882213	1.672577
O	1.519655	5.791369	2.227934
C	-1.465620	4.985311	0.808062
O	-1.861487	5.957286	1.759792
N	0.964358	3.611880	2.064897
C	1.771541	3.172265	3.200785
C	3.186869	2.735966	2.792450
O	4.121871	2.765025	3.603494
C	1.068468	2.038414	3.921931
N	3.337482	2.318050	1.540878
C	4.626439	1.864789	1.049711
C	4.976289	0.426998	1.386249
O	6.152042	0.064384	1.412984
N	3.975371	-0.413965	1.629518
C	4.275810	-1.824306	1.899476
C	3.534785	-2.870116	1.073520
O	4.082805	-3.938281	0.783314
C	4.090591	-2.141754	3.407836
C	5.089950	-1.360034	4.238041
C	2.661827	-1.829555	3.865084
C	2.407522	-2.153398	5.337411
N	2.294956	-2.574437	0.699756
C	1.439084	-3.573991	0.082003
C	1.648074	-3.702581	-1.408919
O	2.220247	-4.689406	-1.894179
N	1.173176	-2.704263	-2.142942
C	1.410533	-2.656178	-3.575901
C	2.909037	-2.485172	-3.877756
O	3.450556	-3.122013	-4.782873
C	0.573782	-1.536479	-4.206497
C	-0.927415	-1.791855	-4.116157
C	-1.746686	-0.549739	-4.437622
N	-1.814711	0.358230	-3.288516
C	-2.547265	1.465695	-3.259972
N	-2.552921	2.237516	-2.173840
N	3.573528	-1.628623	-3.107339
C	5.015125	-1.452502	-3.238876
C	5.727304	-2.785290	-3.045624

O	6.614370	-3.139465	-3.819558
N	-3.277831	1.800308	-4.323512
C	5.530193	-0.417249	-2.232223
O	4.848441	0.817683	-2.400596
O	-0.697240	2.166232	0.117176
O	-0.568146	-0.901112	-1.140502
O	-1.164762	-2.564030	2.235684
C	-0.830482	-3.039655	3.282536
N	-0.894025	-2.379140	4.389191
C	-0.278291	-4.423922	3.363198
H	-5.748066	3.351992	0.344755
H	-4.453702	4.299654	0.646145
H	-5.404347	4.602445	-0.646377
H	-5.850005	0.746974	-3.908246
H	-7.153058	-0.080039	-3.375735
H	-4.513944	-0.387651	-2.393155
H	-5.669438	1.683865	-1.774605
H	-6.701274	0.743544	-0.926433
H	-4.065558	-2.163636	-1.236964
H	-5.654901	-4.403767	-1.334921
H	-4.447898	-4.165462	-0.280780
H	-6.985674	-3.017049	0.319389
H	-6.711525	-4.587106	0.674982
H	-5.556666	-1.263727	1.391916
H	-4.487521	-0.627303	3.409995
H	-3.901734	-2.281806	5.023000
H	-4.408424	-4.569225	4.619935
H	-5.484169	-5.205704	2.600969
H	3.727454	2.998177	-3.000647
H	3.536822	3.236383	-1.396381
H	1.709023	4.118632	-3.399094
H	0.249832	2.546096	-2.234880
H	1.266173	1.991617	-3.386077
H	-0.092955	3.475655	-0.856736
H	0.140702	6.120018	0.185889
H	-2.016180	5.089091	-0.020439
H	-1.605605	4.071582	1.190062
H	-2.828644	5.831964	1.982016
H	0.435568	2.929220	1.560421
H	1.873334	3.958060	3.810922
H	1.624671	1.741290	4.697841
H	0.938567	1.272414	3.292161
H	0.178194	2.353723	4.251129
H	2.549237	2.315142	0.925327
H	4.628541	1.958913	0.054706
H	5.331769	2.455236	1.442603

H	3.029509	-0.089428	1.628632
H	5.229613	-1.908390	1.609701
H	4.253308	-3.119656	3.540769
H	2.490027	-0.854892	3.721499
H	2.026732	-2.366568	3.308817
H	1.461918	-1.928047	5.570072
H	3.028409	-1.616306	5.909138
H	2.566753	-3.127920	5.497141
H	4.959415	-1.573274	5.205971
H	4.951048	-0.380460	4.091747
H	6.018820	-1.609694	3.964486
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H	-1.169719	-2.513980	-4.764697
H	-1.147580	-2.090247	-3.187529
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H	-3.831372	2.633465	-4.307986
H	-3.272268	1.218533	-5.137359
H	-3.105821	3.071208	-2.155430
H	-2.004845	1.983040	-1.376724
H	3.074695	-1.095027	-2.424139
H	5.210521	-1.114577	-4.159945
H	5.375555	-0.755031	-1.303650
H	6.509128	-0.275296	-2.377123
H	5.193876	1.482250	-1.738686
H	5.470502	-3.377594	-2.281498
H	-0.171569	-4.665364	4.328090
H	0.615967	-4.433411	2.915992
H	-1.255759	-1.447015	4.394571
H	-0.581884	-2.799489	5.241174
H	-0.964588	-5.117275	2.879277
H	-6.226210	4.830426	2.166107
H	-5.851777	6.193157	1.086655
H	-7.261623	5.160183	0.758400
H	-5.941132	-0.872080	-4.144471
H	-1.402170	-1.074746	1.751090
H	3.789450	4.517629	-2.388291

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