SUPPORTING INFORMATION

The First Isolated Active Titanium Peroxo Complex: Characterization and Theoretical Study

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Figure S1. ^{31}P NMR spectrum of **1** (0.01 M in MeCN at 20 °C).

Figure S2. Potentiometric titration curve for **1** (0.05 mmol) in MeCN (5 mL) with 0.774 M methanolic TBAOH. The potentials are relative to a standard Ag/AgCl electrode.

Figure S3. UV-vis spectrum of **1** (0.125 mM in MeCN, path length = 1 cm, 20 °C).

DFT xyz structures

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Figure S3. UV-vis spectrum of **1** (0.125 mM in MeCN, path length = 1 cm, 20 °C). λ , nm

DFT xyz structures

[PTiW₁₁O₄₁]⁵⁻. E = -446.2192 eV

P	0.008914	-0.014759	0.013526
Ti	2.774887	2.584913	-0.090549
W	-0.081457	0.070348	3.554291
W	-2.472104	-2.627738	-0.011784
W	-0.085089	0.034611	-3.563957
W	3.117717	-0.389793	1.653031
W	0.473880	-3.111461	-1.712420
W	-2.994259	0.612204	-1.821359
W	-0.731051	3.021312	1.877548
W	-3.059680	0.501164	1.888845
W	-0.462253	2.993946	-1.857313
W	3.131339	-0.449821	-1.729018
W	0.476947	-3.083592	1.713636
O	1.549293	0.236340	-0.004395
O	-0.680270	0.628389	1.290314
O	-0.306708	-1.570562	0.009377
O	-0.635220	0.636802	-1.276782
O	-0.940291	3.286036	0.045793
O	2.063253	-2.085637	1.619914
O	-3.306598	0.955045	0.053809
O	2.056532	-2.130680	-1.610549
O	-0.144946	-1.734762	2.958343
O	1.710580	0.055036	-2.969745
O	-2.933794	-1.298454	1.335819
O	1.280352	2.888857	-1.297340
O	-2.895977	-1.244194	-1.269241
O	1.253485	2.853150	1.476823
O	-0.177504	-1.764361	-2.929722
O	1.678981	0.166677	2.850446
O	3.879244	-0.954047	0.006364
O	-2.489223	2.367657	2.154113
O	0.854637	-3.914950	0.008027
O	-2.348198	2.393832	-2.023135
O	3.573634	1.292249	-1.427739
O	-1.406541	-3.491917	1.337617
O	-0.134070	1.980349	-3.453051
O	-2.022606	0.100053	3.455372
O	-0.198657	2.015009	3.452672
O	-2.027073	0.127071	-3.409394
O	3.515782	1.397634	1.301174
O	-1.410951	-3.517086	-1.328976
O	4.163627	3.711748	-0.623645
O	3.347104	4.300073	0.425214
O	0.175183	-0.107435	5.262341
O	-3.905080	-3.608639	-0.020894
O	0.087622	-0.184546	-5.276284
O	4.381647	-0.828823	2.763259
O	0.875784	-4.418775	-2.782308
O	-4.604300	0.740472	-2.457609
O	-0.857078	4.627158	2.521269
O	-4.668832	0.575359	2.534596
O	-0.586609	4.601248	-2.498705
O	4.393098	-0.967855	-2.805629
O	0.891000	-4.381597	2.789717

[HPTiW₁₁O₄₁]⁴⁻. E = -456.2058 eV

P	0.008914	-0.014759	0.013526
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