Electronic Supporting Information

Protonation state of the macrocyclic $\{H_nP_8W_{48}O_{184}\}$ anion by modeling of ^{183}W NMR chemical shifts.

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Fig. S1. ^{183}W NMR spectra in 1 M LiCl D_2O solution of 2.2 mM $(NH_4)_{21}Li_{17}H_2[P_8W_{48}O_{184}]$ at a) pH 1.1, b) pH 1.8, c) pH 2.9, d) pH 3.7, e) pH 4.7, f) pH 5.9 and e) pH 7.6.

Fig. S2. ^{183}W NMR chemical shifts of $(NH_4)_{21}Li_{17}H_2[P_8W_{48}O_{184}]$ as a function of a) pH and b) the molar ratio H/POT.

Table S1. Cartesian coordinates for $[P_2W_{18}O_{62}]^{6-}$ in H_2O.

Table S2. Cartesian coordinates for β-$[SiW_{12}O_{40}]^{4-}$ in H_2O.

Table S3. Cartesian coordinates for β-$[SiW_{12}O_{40}]^{4-}$ in DMF.

Table S4. Cartesian coordinates for γ-$[SiW_{12}O_{40}]^{4-}$ in DMF.

Table S5. Cartesian coordinates for $[W_{10}O_{32}]^{4-}$ in DMF.

Table S6. Cartesian coordinates for $[8K]\subset[H_{16}P_8W_{48}O_{184}]^{16-}$.

Table S7. Computed parameters to calculate ^{183}W chemical shifts relative to WO_4^{2-} for $[8K]\subset[H_nP_8W_{48}O_{184}]^{(32-n)-}$.

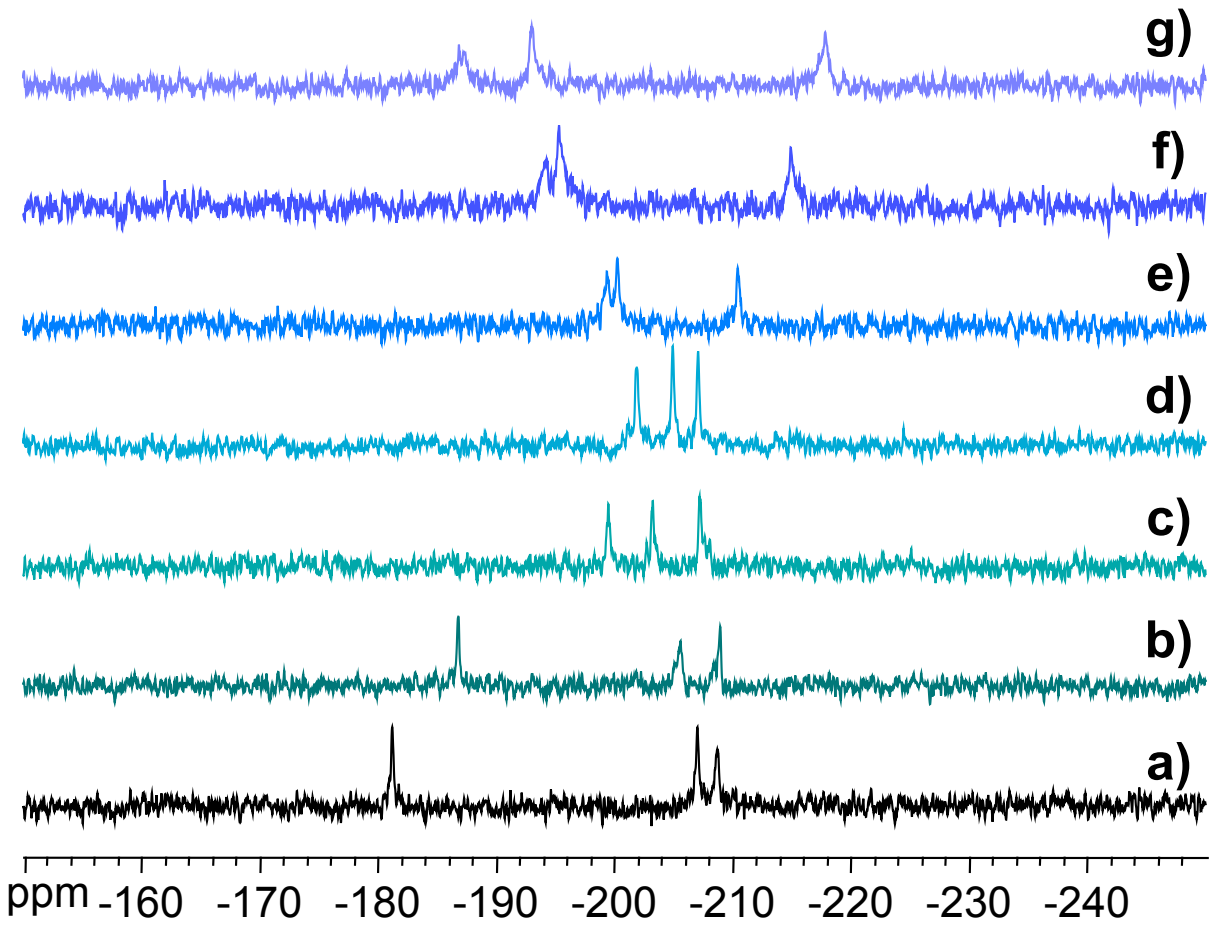

Fig. S1. ^{183}W NMR spectra in 1 M LiCl D_2O solution of 2.2 mM $(NH_4)_{21}Li_{17}H_2[P_8W_{48}O_{184}]$ at a) pH 1.1, b) pH 1.8, c) pH 2.9, d) pH 3.7, e) pH 4.7, f) pH 5.9 and e) pH 7.6.

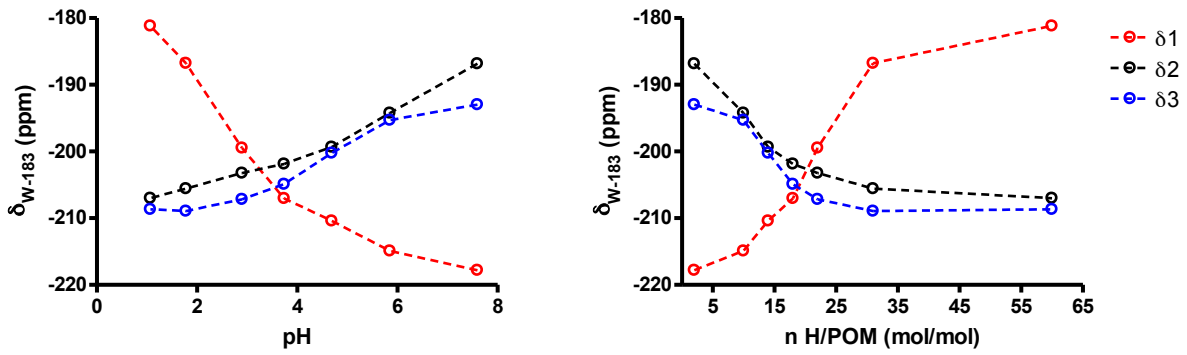

Fig. S2. ^{183}W NMR chemical shifts of $(NH_4)_{21}Li_{17}H_2[P_8W_{48}O_{184}]$ as a function of a) pH and b) the molar ratio H/POT.

Table S1. Cartesian coordinates for $[P_2W_{18}O_{62}]^{6-}$ in H_2O*

82

W1	-3.136340	-1.707846	-1.898202
W2	-3.136340	-1.707846	1.898202
W3	-3.136340	1.707846	-1.898202
W4	-3.136340	1.707846	1.898202
W5	3.047208	-1.862227	-1.898202
W6	3.047208	-1.862227	1.898202
W7	3.047208	1.862227	-1.898202
W8	3.047208	1.862227	1.898202
W9	0.089132	-3.570073	-1.898202
W10	0.089132	-3.570073	1.898202
W11	0.089132	3.570073	-1.898202
W12	0.089132	3.570073	1.898202
W13	1.985306	0.000000	-4.973358
W14	1.985306	0.000000	4.973358
W15	-0.992653	-1.719325	-4.973358
W16	-0.992653	-1.719325	4.973358
W17	-0.992653	1.719325	-4.973358
W18	-0.992653	1.719325	4.973358
P19	0.000000	0.000000	-2.012007
P20	0.000000	0.000000	2.012007
O21	-4.458050	-2.780049	-2.230257
O22	-4.458050	-2.780049	2.230257
O23	-4.458050	2.780049	-2.230257
O24	-4.458050	2.780049	2.230257
O25	-4.004482	0.000000	-2.158487
O26	-4.004482	0.000000	2.158487
O27	-3.365825	-1.545223	0.000000
O28	-3.365825	1.545223	0.000000
O29	-2.435524	-1.617555	-3.711975
O30	-2.435524	-1.617555	3.711975
O31	-2.435524	1.617555	-3.711975
O32	-2.435524	1.617555	3.711975
O33	-1.685250	-2.918938	-1.563623
O34	-1.685250	-2.918938	1.563623
O35	-1.685250	2.918938	-1.563623
O36	-1.685250	2.918938	1.563623
O37	-1.618664	-2.803609	-6.172828
O38	-1.618664	-2.803609	6.172828
O39	-1.618664	2.803609	-6.172828
O40	-1.618664	2.803609	6.172828
O41	-1.547062	0.000000	-5.695941
O42	-1.547062	0.000000	5.695941
O43	-1.483117	0.000000	-1.544007
O44	-1.483117	0.000000	1.544007
O45	-0.183082	-2.918003	-3.711975
O46	-0.183082	-2.918003	3.711975
O47	-0.183082	2.918003	-3.711975

O48	-0.183082	2.918003	3.711975
O49	-0.178568	-5.250809	-2.230257
O50	-0.178568	-5.250809	2.230257
O51	-0.178568	5.250809	-2.230257
O52	-0.178568	5.250809	2.230257
O53	4.636618	-2.470760	-2.230257
O54	4.636618	-2.470760	2.230257
O55	4.636618	2.470760	-2.230257
O56	4.636618	2.470760	2.230257
O57	3.370499	0.000000	-1.563623
O58	3.370499	0.000000	1.563623
O59	3.237329	0.000000	-6.172828
O60	3.237329	0.000000	6.172828
O61	3.021115	-2.142279	0.000000
O62	3.021115	2.142279	0.000000
O63	2.618606	-1.300448	-3.711975
O64	2.618606	-1.300448	3.711975
O65	2.618606	1.300448	-3.711975
O66	2.618606	1.300448	3.711975
O67	2.002241	-3.467983	-2.158487
O68	2.002241	-3.467983	2.158487
O69	2.002241	3.467983	-2.158487
O70	2.002241	3.467983	2.158487
O71	0.773531	-1.339795	-5.695941
O72	0.773531	-1.339795	5.695941
O73	0.773531	1.339795	-5.695941
O74	0.773531	1.339795	5.695941
O75	0.741558	-1.284417	-1.544007
O76	0.741558	-1.284417	1.544007
O77	0.741558	1.284417	-1.544007
O78	0.741558	1.284417	1.544007
O79	0.344710	-3.687502	0.000000
O80	0.344710	3.687502	0.000000
O81	0.000000	0.000000	-3.609332
O82	0.000000	0.000000	3.609332

* from Ref 16: Vila-Nadal, L.; Sarasa, J. P.; Rodriguez-Fortea, A.; Igual, J.; Kazansky, L. P.; Poblet, J. M. *Chem.-Asian J.* **2010**, *5*, 97-104.

Table S2. Cartesian coordinates for β-$[SiW_{12}O_{40}]^{4-}$ in H_2O*

53

Si1	0.000000	0.000000	0.000548
W2	1.076005	1.863696	-2.860965
W3	-2.152011	0.000000	-2.860965
W4	1.076005	-1.863696	-2.860965
W5	-3.153615	1.679970	-0.069004
W6	3.031704	-1.891126	-0.069004
W7	0.121911	3.571095	-0.069004
W8	0.121911	-3.571095	-0.069004
W9	-3.153615	-1.679970	-0.069004
W10	3.031704	1.891126	-0.069004
W11	-1.965614	0.000000	2.995605
W12	0.982807	-1.702272	2.995605
W13	0.982807	1.702272	2.995605
O14	0.772266	1.337604	-0.550167
O15	-1.544532	0.000000	-0.550167
O16	0.000000	0.000000	1.638736
O17	0.772266	-1.337604	-0.550167
O18	-0.746571	-1.293100	-3.059254
O19	0.166940	2.921051	1.744921
O20	-1.651893	-2.861163	-0.252398
O21	2.446234	1.605100	1.744921
O22	-2.613175	1.315951	1.744921
O23	3.303787	0.000000	-0.252398
O24	-2.613175	-1.315951	1.744921
O25	1.493143	0.000000	-3.059254
O26	0.166940	-2.921051	1.744921
O27	-0.746571	1.293100	-3.059254
O28	2.446234	-1.605100	1.744921
O29	-1.651893	2.861163	-0.252398
O30	2.051865	3.553935	0.071111
O31	-3.203749	-1.367549	-1.978771
O32	-0.773812	1.340281	3.721025
O33	0.417543	-3.458303	-1.978771
O34	2.786206	2.090754	-1.978771
O35	-0.773812	-1.340281	3.721025
O36	2.786206	-2.090754	-1.978771
O37	-4.103731	0.000000	0.071111
O38	-3.203749	1.367549	-1.978771
O39	2.051865	-3.553935	0.071111
O40	0.417543	3.458303	-1.978771
O41	1.547623	0.000000	3.721025
O42	1.436061	2.487330	-4.431442
O43	-4.458170	2.794545	0.134324
O44	1.605732	-2.781210	4.192213
O45	4.649232	-2.463616	0.134324
O46	-0.191062	5.258161	0.134324
O47	1.605732	2.781210	4.192213

O48	-0.191062	-5.258161	0.134324
O49	-2.872121	0.000000	-4.431442
O50	-4.458170	-2.794545	0.134324
O51	1.436061	-2.487330	-4.431442
O52	4.649232	2.463616	0.134324
O53	-3.211464	0.000000	4.192213

* from Ref 16: Vila-Nadal, L.; Sarasa, J. P.; Rodriguez-Fortea, A.; Igual, J.; Kazansky, L. P.; Poblet, J. M. *Chem.-Asian J.* **2010**, *5*, 97-104.

Table S3. Cartesian coordinates for β-$[SiW_{12}O_{40}]^{4-}$ (DMF)*

53

Si1	0.000000	0.000000	0.000583
W2	1.076029	1.863738	-2.861009
W3	-2.152059	0.000000	-2.861009
W4	1.076029	-1.863738	-2.861009
W5	-3.153667	1.679954	-0.069005
W6	3.031717	-1.891179	-0.069005
W7	0.121950	3.571133	-0.069005
W8	0.121950	-3.571133	-0.069005
W9	-3.153667	-1.679954	-0.069005
W10	3.031717	1.891179	-0.069005
W11	-1.965635	0.000000	2.995658
W12	0.982817	-1.702290	2.995658
W13	0.982817	1.702290	2.995658
O14	0.772282	1.337632	-0.550180
O15	-1.544565	0.000000	-0.550180
O16	0.000000	0.000000	1.638764
O17	0.772282	-1.337632	-0.550180
O18	-0.746590	-1.293132	-3.059356
O19	0.166954	2.921122	1.744934
O20	-1.651939	-2.861242	-0.252411
O21	2.446289	1.605148	1.744934
O22	-2.613243	1.315974	1.744934
O23	3.303878	0.000000	-0.252411
O24	-2.613243	-1.315974	1.744934
O25	1.493181	0.000000	-3.059356
O26	0.166954	-2.921122	1.744934
O27	-0.746590	1.293132	-3.059356
O28	2.446289	-1.605148	1.744934
O29	-1.651939	2.861242	-0.252411
O30	2.051902	3.553998	0.071101
O31	-3.203851	-1.367561	-1.978838
O32	-0.773816	1.340289	3.721123
O33	0.417583	-3.458397	-1.978838
O34	2.786268	2.090835	-1.978838
O35	-0.773816	-1.340289	3.721123
O36	2.786268	-2.090835	-1.978838
O37	-4.103804	0.000000	0.071101
O38	-3.203851	1.367561	-1.978838
O39	2.051902	-3.553998	0.071101
O40	0.417583	3.458397	-1.978838
O41	1.547633	0.000000	3.721123
O42	1.436112	2.487419	-4.431552
O43	-4.458296	2.794598	0.134330
O44	1.605758	-2.781255	4.192335
O45	4.649341	-2.463699	0.134330
O46	-0.191045	5.258297	0.134330
O47	1.605758	2.781255	4.192335

O48	-0.191045	-5.258297	0.134330
O49	-2.872224	0.000000	-4.431552
O50	-4.458296	-2.794598	0.134330
O51	1.436112	-2.487419	-4.431552
O52	4.649341	2.463699	0.134330
O53	-3.211517	0.000000	4.192335

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Table S4. Cartesian coordinates for γ-$[SiW_{12}O_{40}]^{4-}$ (DMF)*

53

Si1	0.000000	0.000000	0.000625
W2	1.519049	0.000000	3.517011
W3	-1.519049	0.000000	3.517011
W4	0.000000	3.563319	-0.173331
W5	0.000000	-3.563319	-0.173331
W6	2.983336	1.687045	0.896882
W7	-2.983336	1.687045	0.896882
W8	-2.983336	-1.687045	0.896882
W9	2.983336	-1.687045	0.896882
W10	1.695793	-1.892768	-2.547251
W11	-1.695793	-1.892768	-2.547251
W12	-1.695793	1.892768	-2.547251
W13	1.695793	1.892768	-2.547251
O14	0.000000	1.217281	3.421290
O15	0.000000	-1.217281	3.421290
O16	1.755133	0.000000	-2.841552
O17	-1.755133	0.000000	-2.841552
O18	1.438551	-2.875551	0.871606
O19	-1.438551	-2.875551	0.871606
O20	-1.438551	2.875551	0.871606
O21	1.438551	2.875551	0.871606
O22	2.836374	-1.604943	-0.995975
O23	2.836374	1.604943	-0.995975
O24	-2.836374	-1.604943	-0.995975
O25	-2.836374	1.604943	-0.995975
O26	0.000000	-2.009776	-3.470298
O27	0.000000	2.009776	-3.470298
O28	2.624674	-1.369825	2.795371
O29	-2.624674	-1.369825	2.795371
O30	-2.624674	1.369825	2.795371
O31	2.624674	1.369825	2.795371
O32	3.928145	0.000000	0.903067
O33	-3.928145	0.000000	0.903067
O34	-1.265952	-3.540397	-1.665054
O35	1.265952	-3.540397	-1.665054
O36	-1.265952	3.540397	-1.665054
O37	1.265952	3.540397	-1.665054
O38	-1.928286	0.000000	5.194121
O39	1.928286	0.000000	5.194121
O40	2.799810	2.460372	-3.748750
O41	-2.799810	-2.460372	-3.748750
O42	-2.799810	2.460372	-3.748750
O43	2.799810	-2.460372	-3.748750
O44	4.289435	-2.805097	1.071806
O45	-4.289435	-2.805097	1.071806
O46	-4.289435	2.805097	1.071806
O47	4.289435	2.805097	1.071806

O48	0.000000	-5.243124	0.235535
O49	0.000000	5.243124	0.235535
O50	0.000000	-1.337347	-0.969176
O51	0.000000	1.337347	-0.969176
O52	-1.352255	0.000000	0.929991
O53	1.352255	0.000000	0.929991

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Table S5. Cartesian coordinates for $[W_{10}O_{32}]^{4-}$ (DMF)*

42			
W	2.345892	0.000000	1.909503
W	-2.345892	0.000000	1.909503
W	2.345892	0.000000	-1.909503
W	-2.345892	0.000000	-1.909503
W	0.000000	2.345892	1.909503
W	0.000000	-2.345892	1.909503
W	0.000000	2.345892	-1.909503
W	0.000000	-2.345892	-1.909503
W	0.000000	0.000000	4.278590
W	0.000000	0.000000	-4.278590
O	0.000000	0.000000	1.934162
O	0.000000	0.000000	-1.934162
O	1.875500	1.875500	1.891218
O	-1.875500	1.875500	1.891218
O	1.875500	-1.875500	1.891218
O	-1.875500	-1.875500	1.891218
O	1.875500	1.875500	-1.891218
O	-1.875500	1.875500	-1.891218
O	1.875500	-1.875500	-1.891218
O	-1.875500	-1.875500	-1.891218
O	0.000000	1.873195	3.812005
O	0.000000	-1.873195	3.812005
O	0.000000	1.873195	-3.812005
O	0.000000	-1.873195	-3.812005
O	0.000000	2.285599	0.000000
O	0.000000	-2.285599	0.000000
O	1.873195	0.000000	3.812005
O	-1.873195	0.000000	3.812005
O	1.873195	0.000000	-3.812005
O	-1.873195	0.000000	-3.812005
O	2.285599	0.000000	0.000000
O	-2.285599	0.000000	0.000000
O	4.061944	0.000000	2.145018
O	-4.061944	0.000000	2.145018
O	4.061944	0.000000	-2.145018
O	-4.061944	0.000000	-2.145018
O	0.000000	0.000000	6.017610
O	0.000000	0.000000	-6.017610
O	0.000000	4.061944	2.145018
O	0.000000	-4.061944	2.145018
O	0.000000	4.061944	-2.145018
O	0.000000	-4.061944	-2.145018

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Table S6. Cartesian coordinates for $[8K]\subset[H_{16}P_8W_{48}O_{184}]^{16-}$

264

W	5.25483	-18.87234	-19.73284
W	21.52547	-7.90795	-19.73284
W	18.87234	-21.52547	-19.73284
W	7.90795	-5.25483	-19.73284
W	5.25483	-7.90795	-19.73284
W	21.52547	-18.87234	-19.73284
W	18.87234	-5.25483	-19.73284
W	7.90795	-21.52547	-19.73284
W	21.52547	-18.87234	-23.09016
W	5.25483	-7.90795	-23.09016
W	7.90795	-21.52547	-23.09016
W	18.87234	-5.25483	-23.09016
W	21.52547	-7.90795	-23.09016
W	5.25483	-18.87234	-23.09016
W	7.90795	-5.25483	-23.09016
W	18.87234	-21.52547	-23.09016
W	7.61953	-16.47604	-18.03662
W	19.16076	-10.30425	-18.03662
W	16.47604	-19.16076	-18.03662
W	10.30425	-7.61953	-18.03662
W	7.61953	-10.30425	-18.03662
W	19.16076	-16.47604	-18.03662
W	16.47604	-7.61953	-18.03662
W	10.30425	-19.16076	-18.03662
W	19.16076	-16.47604	-24.78638
W	7.61953	-10.30425	-24.78638
W	10.30425	-19.16076	-24.78638
W	16.47604	-7.61953	-24.78638
W	19.16076	-10.30425	-24.78638
W	7.61953	-16.47604	-24.78638
W	10.30425	-7.61953	-24.78638
W	16.47604	-19.16076	-24.78638
W	4.55479	-15.24013	-19.73905
W	22.22550	-11.54016	-19.73905
W	15.24013	-22.22550	-19.73905
W	11.54016	-4.55479	-19.73905
W	4.55479	-11.54016	-19.73905
W	22.22550	-15.24013	-19.73905
W	15.24013	-4.55479	-19.73905
W	11.54016	-22.22550	-19.73905
W	22.22550	-15.24013	-23.08395
W	4.55479	-11.54016	-23.08395
W	11.54016	-22.22550	-23.08395
W	15.24013	-4.55479	-23.08395
W	22.22550	-11.54016	-23.08395
W	4.55479	-15.24013	-23.08395
W	11.54016	-4.55479	-23.08395

W	15.24013	-22.22550	-23.08395
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P	10.17464	-19.55230	-21.41150
P	16.60566	-7.22800	-21.41150
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O	19.55230	-22.65881	-18.62372
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O	4.12149	-7.22800	-18.62372
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O	7.22800	-22.65881	-18.62372
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O	7.22800	-22.65881	-24.19928
O	19.55230	-4.12149	-24.19928
O	22.65881	-7.22800	-24.19928
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O	22.39368	-9.61680	-19.85489
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O	9.61680	-22.39368	-19.85489
O	22.39368	-17.16349	-22.96812

O	4.38661	-9.61680	-22.96812
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O	22.39368	-9.61680	-22.96812
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O	8.77322	-20.25126	-21.41150
O	18.00707	-6.52904	-21.41150
O	6.52904	-18.00707	-21.41150
O	20.25126	-8.77322	-21.41150
O	18.00707	-20.25126	-21.41150
O	8.77322	-6.52904	-21.41150
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O	19.62996	-10.16045	-16.36909
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O	10.16045	-7.15034	-16.36909
O	7.15034	-10.16045	-16.36909
O	19.62996	-16.61985	-16.36909
O	16.61985	-7.15034	-16.36909
O	10.16045	-19.62996	-16.36909
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O	7.15034	-10.16045	-26.45391
O	10.16045	-19.62996	-26.45391
O	16.61985	-7.15034	-26.45391
O	19.62996	-10.16045	-26.45391
O	7.15034	-16.61985	-26.45391
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O	16.61985	-19.62996	-26.45391
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O	18.22667	-11.81011	-17.97067
O	14.97019	-18.22667	-17.97067

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O	14.97019	-8.55363	-17.97067
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O	20.75473	-15.50311	-18.60445
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O	20.75473	-15.50311	-24.21855
O	6.02557	-11.27718	-24.21855
O	11.27718	-20.75473	-24.21855
O	15.50311	-6.02557	-24.21855
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O	8.04480	-10.37469	-22.66836
O	10.37469	-18.73549	-22.66836
O	16.40561	-8.04480	-22.66836
O	18.73549	-10.37469	-22.66836

O	8.04480	-16.40561	-22.66836
O	10.37469	-8.04480	-22.66836
O	16.40561	-18.73549	-22.66836
O	3.24845	-14.94340	-18.68368
O	23.53185	-11.83689	-18.68368
O	14.94340	-23.53185	-18.68368
O	11.83689	-3.24845	-18.68368
O	3.24845	-11.83689	-18.68368
O	23.53185	-14.94340	-18.68368
O	14.94340	-3.24845	-18.68368
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O	23.53185	-14.94340	-24.13932
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O	11.83689	-23.53185	-24.13932
O	14.94340	-3.24845	-24.13932
O	23.53185	-11.83689	-24.13932
O	3.24845	-14.94340	-24.13932
O	11.83689	-3.24845	-24.13932
O	14.94340	-23.53185	-24.13932
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O	11.72441	-23.15960	-21.41150
O	15.05588	-3.62070	-21.41150
O	3.62070	-15.05588	-21.41150
O	23.15960	-11.72441	-21.41150
O	15.05588	-23.15960	-21.41150
O	11.72441	-3.62070	-21.41150
O	20.68242	-15.52722	-21.41150
O	6.09787	-11.25308	-21.41150
O	11.25308	-20.68242	-21.41150
O	15.52722	-6.09787	-21.41150
O	6.09787	-15.52722	-21.41150
O	20.68242	-11.25308	-21.41150
O	15.52722	-20.68242	-21.41150
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K	18.93367	-13.39015	-21.41150
K	7.84663	-13.39015	-21.41150
K	13.39015	-18.93367	-21.41150
K	13.39015	-7.84663	-21.41150
K	10.61839	-16.16191	-21.41150
K	10.61839	-10.61839	-21.41150
K	16.16191	-16.16191	-21.41150

K	16.16191	-10.61839	-21.41150
H	8.58911	-14.65154	-17.05519
H	18.19119	-12.12876	-17.05519
H	14.65154	-18.19119	-17.05519
H	12.12876	-8.58911	-17.05519
H	8.58911	-12.12876	-17.05519
H	18.19119	-14.65154	-17.05519
H	14.65154	-8.58911	-17.05519
H	12.12876	-18.19119	-17.05519
H	18.19119	-14.65154	-25.76781
H	8.58911	-12.12876	-25.76781
H	12.12876	-18.19119	-25.76781
H	14.65154	-8.58911	-25.76781
H	18.19119	-12.12876	-25.76781
H	8.58911	-14.65154	-25.76781
H	12.12876	-8.58911	-25.76781
H	14.65154	-18.19119	-25.76781

Table S7. Computed parameters to calculate ^{183}W chemical shifts relative to WO_4^{2-} for $[8K]\subset[H_nP_8W_{48}O_{184}]^{(32-n)-}$.

$[8K]\subset[H_nP_8W_{48}O_{184}]^{(32-n)-}$	Site	Computed parameters by PACHA							Experimental data	
		ΔE^a (eV)	q(W)	$<(a_0/r)^3>^b$ (au)	$P_u{}^c$	$\sigma_{para}{}^d$ (ppm)	σ_{dia} (ppm)	$\delta_{PACHA}{}^e$ (ppm)	δ_{exp} (ppm)	pH
$[8K]\subset[H_{16}P_8W_{48}O_{184}]^{16-}$	W3	3.312	1.874031	9.014081	1.56054	-8654.7	8689.0	-210.2	-207.7	1.1
	W1		1.856221	8.928431	1.56884	-8661.6	8689.2	-203.4	-205.9	
	W2		1.753771	8.435641	1.61510	-8684.8	8690.0	-181.0	-180.9	
$[8K]\subset[H_{15}P_8W_{48}O_{184}]^{17-}$	W3	3.313	1.860481	8.948931	1.56686	-8657.0	8689.1	-207.9	-208.5	1.3
	W1		1.847441	8.886211	1.57291	-8661.7	8689.2	-203.4	-203.9	
	W2		1.742811	8.382921	1.61989	-8682.7	8690.1	-183.2	-182.7	
$[8K]\subset[H_{14}P_8W_{48}O_{184}]^{18-}$	W3	3.314	1.846941	8.883791	1.57314	-8659.2	8689.2	-205.8		
	W1		1.838481	8.843101	1.57704	-8661.9	8689.3	-203.2		
	W2		1.731781	8.329861	1.62469	-8680.6	8690.2	-185.4		
$[8K]\subset[H_{13}P_8W_{48}O_{184}]^{19-}$	W3	3.315	1.833351	8.818401	1.57940	-8661.2	8689.4	-203.9		
	W1		1.829411	8.799471	1.58120	-8662.4	8689.4	-202.8		
	W2		1.720631	8.276251	1.62950	-8678.5	8690.2	-187.5		
$[8K]\subset[H_{12}P_8W_{48}O_{184}]^{20-}$	W3	3.316	1.819741	8.752961	1.58561	-8663.1	8689.5	-202.2	-199.8	2.2
	W1		1.820181	8.755081	1.58541	-8662.9	8689.5	-202.3	-206.2	
	W2		1.709521	8.222791	1.63426	-8676.4	8690.3	-189.7	-189.7	
$[8K]\subset[H_{11}P_8W_{48}O_{184}]^{21-}$	W3	3.316	1.806151	8.687561	1.59178	-8664.7	8689.6	-200.6		
	W1		1.810591	8.708951	1.58976	-8663.6	8689.5	-201.7		
	W2		1.698371	8.169171	1.63902	-8674.4	8690.4	-191.9		
$[8K]\subset[H_{10}P_8W_{48}O_{184}]^{22-}$	W3	3.317	1.792481	8.621841	1.59793	-8666.3	8689.7	-199.2		
	W1		1.800891	8.662281	1.59415	-8664.5	8689.6	-200.9		
	W2		1.687131	8.115081	1.64378	-8672.3	8690.5	-194.0		
$[8K]\subset[H_9P_8W_{48}O_{184}]^{23-}$	W3	3.317	1.778871	8.556381	1.60401	-8667.6	8689.8	-198.0	-197.8	3.1
	W1		1.790871	8.614101	1.59864	-8665.5	8689.7	-200.0	-202.5	
	W2		1.675991	8.061521	1.64846	-8670.3	8690.6	-196.1	-196.5	
$[8K]\subset[H_8P_8W_{48}O_{184}]^{24-}$	W3	3.318	1.765211	8.490631	1.61007	-8668.9	8689.9	-196.8		
	W1		1.780741	8.565331	1.60317	-8666.6	8689.8	-199.0		
	W2		1.664781	8.007591	1.65315	-8668.3	8690.7	-198.2		
$[8K]\subset[H_7P_8W_{48}O_{184}]^{25-}$	W3	3.318	1.751551	8.424941	1.61607	-8670.0	8690.0	-195.8		
	W1		1.770661	8.516851	1.60765	-8667.7	8689.9	-197.9		
	W2		1.653501	7.953351	1.65783	-8666.3	8690.8	-200.2		
$[8K]\subset[H_6P_8W_{48}O_{184}]^{26-}$	W3	3.318	1.737851	8.359051	1.62205	-8670.9	8690.1	-195.0	-194.2	4.0
	W1		1.760461	8.467811	1.61215	-8669.0	8689.9	-196.7	-198.9	
	W2		1.642231	7.899101	1.66248	-8664.4	8690.9	-202.3	-202.2	

$[8K]\subset[H_5P_8W_{48}O_{184}]^{27-}$	W3	3.318	1.724	1318.29	309	1.62799	-8671.8	8690.2	-194.2		
	W1		1.750	1018.41	800	1.61670	-8670.4	8690.0	-195.4		
	W2		1.630	9017.84	463	1.66711	-8662.5	8691.0	-204.3		
$[8K]\subset[H_4P_8W_{48}O_{184}]^{28-}$	W3	3.317	1.710	5018.22	751	1.63385	-8672.5	8690.3	-193.6		
	W1		1.739	4518.36	675	1.62135	-8671.9	8690.1	-194.0		
	W2		1.619	6517.79	049	1.67169	-8660.6	8691.0	-206.2		
$[8K]\subset[H_3P_8W_{48}O_{184}]^{29-}$	W3	3.317	1.696	7518.16	135	1.63971	-8673.1	8690.4	-193.1	-193.9	5.0
	W1		1.728	4918.31	402	1.62610	-8673.4	8690.2	-192.6	-191.4	
	W2		1.608	3217.73	603	1.67626	-8658.8	8691.1	-208.1	-206.3	
$[8K]\subset[H_2P_8W_{48}O_{184}]^{30-}$	W3	3.316	1.683	0018.09	521	1.64552	-8673.6	8690.5	-192.7	-193.3	5.8
	W1		1.717	2918.26	015	1.63093	-8675.1	8690.3	-191.0	-191.1	
	W2		1.597	0017.68	159	1.68080	-8657.1	8691.2	-210.0	-208.5	
$[8K]\subset[HP_8W_{48}O_{184}]^{31-}$	W3	3.316	1.669	2318.02	899	1.65129	-8674.0	8690.7	-192.4		
	W1		1.705	8518.20	514	1.63583	-8676.7	8690.4	-189.4		
	W2		1.585	7117.62	726	1.68530	-8655.4	8691.3	-211.7		
$[8K]\subset[P_8W_{48}O_{184}]^{32-}$	W3	3.315	1.655	4517.96	273	1.65702	-8674.3	8690.8	-192.2		
	W1		1.694	1718.14	894	1.64080	-8678.5	8690.5	-187.8		
	W2		1.574	4917.57	331	1.68973	-8653.8	8691.4	-213.4		

[a] calculated for δ_{mean} = -20.6 ppm. [b] calculated according to eq (5) with f = 0.481 and efg° = 10 au. [c] calculated according to eq (4). [d] calculated according to eq (2b). [e] calculated according to eq (1) with σ_{ref} = -175.8 ppm.