

Electronic Supplementary Information for PCCP article

**Charge Retention of Soft-Landed Phosphotungstate Keggin Anions on Self-Assembled
Monolayers**

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Table S1. Calculated vibrational frequencies of WPOM³⁻, WPOM²⁻, WPOM¹⁻, and WPOM⁰ in the 1200-800 cm⁻¹ range.

WPOM ³⁻		WPOM ²⁻		WPOM ¹⁻		WPOM ⁰		Assignment
Frequency [cm ⁻¹]	Intensity [KM/mol]	Frequency [cm ⁻¹]	Intensity [KM/mol]	Frequency [cm ⁻¹]	Intensity [KM/mol]	Frequency [cm ⁻¹]	Intensity [KM/mol]	
817.7	2636.6	783.1	1784.7	785.3	1751.93	779.0	1997.42	W-Ob1-W stretch with contribution from W-Ob1-W & W=Ot
817.9	2608.2	823.4	2395.3	814.0	2016.96	819.6	1959.31	W-Ob1-W stretch with contribution from W-Ob1-W & W=Ot
818.3	2565.9	827.8	2506.5	829.3	2122.92	826.7	1753.21	W-Ob1-W stretch with contribution from W-Ob1-W & W=Ot
888.0	543.5	885.2	331.8	849.7	342.44	837.7	642.38	W-Ob2-W stretch with contribution from W-Ob2-W & W=Ot
888.3	538.3	890.3	857.0	890.5	403.95	858.3	264.97	W-Ob2-W stretch with contribution from W-Ob2-W & W=Ot
888.5	544.9	898.0	429.9	894.4	626.24	892.9	303.63	W-Ob2-W stretch with contribution from W-Ob2-W & W=Ot
903.8	0.2	902.2	132.9	907.7	67.54	906.4	308.17	W-Ob2-W and W-Ob1-W stretch with contribution from W=Ot
904.0	0.4	910.1	36.8	913.6	169.40	917.0	152.39	W-Ob2-W and W-Ob1-W stretch with contribution from W=Ot
904.2	0.5	914.3	41.9	917.6	37.30	922.1	75.03	W-Ob2-W and W-Ob1-W stretch with contribution from W=Ot
907.9	0.1	919.9	0.1	923.5	10.05	932.4	53.44	W-Ob2-W and W-Ob1-W stretch
908.1	0.1	920.3	23.8	925.3	23.57			W-Ob2-W and W-Ob1-W stretch
964.3	233.3	965.1	4.8	958.6	14.92	958.7	19.98	asym W=Ot stretch with P-O stretch
965.6	307.0	979.5	629.3	990.5	801.15	1002.5	838.64	partial asym W=Ot stretch with contribution from P-O stretch
966.6	512.4	980.2	691.0	991.2	800.84	1002.8	729.28	partial asym W=Ot stretch with contribution from P-O stretch
966.8	548.3	981.3	663.2	993.5	746.56	1004.6	645.22	partial asym W=Ot stretch with contribution from P-O stretch
974.0	456.7	988.9	166.2	1004.6	57.96	1018.7	93.50	asym W=Ot stretch
974.1	476.2	989.7	183.9	1004.8	40.46	1020.0	7.69	asym W=Ot stretch
974.5	422.8	991.5	66.9	1006.0	94.36	1020.6	23.53	asym W=Ot stretch
974.6	14.7	992.2	225.6	1006.4	146.03	1021.6	187.35	asym W=Ot stretch
974.9	23.9	992.5	267.2	1007.0	155.69	1022.1	272.46	asym W=Ot stretch
975.1	40.3	993.0	125.4	1007.2	146.85	1023.2	103.92	asym W=Ot stretch
975.5	7.5	993.2	266.8	1007.5	274.42	1023.6	142.50	asym W=Ot stretch
975.9	8.2	993.6	43.9	1007.9	194.46	1024.2	104.26	asym W=Ot stretch
991.7	0.1	1008.4	4.4	1020.9	1.02	1033.9	0.16	sym W=Ot stretch
1057.8	356.5	1056.771	268.1	1051.9	108.56	1054.95	73.66	PO4 asym with partial W=Ot stretch

1058.5	357.1	1059.558	280.3	1057.2	179.46	1058.192	83.84	PO4 asym with partial W=Ot stretch
1059.1	346.3	1061.024	288.9	1064.8	146.60	1062.166	103.35	PO4 asym with partial W=Ot stretch