Supporting Informations

Encapsulation of two Potassium Cations in Preyssler-type Phosphotungstates: Preparation, Structural Characterization, Thermal Stability, Activity as an Acid Catalyst, and HAADF-STEM images.

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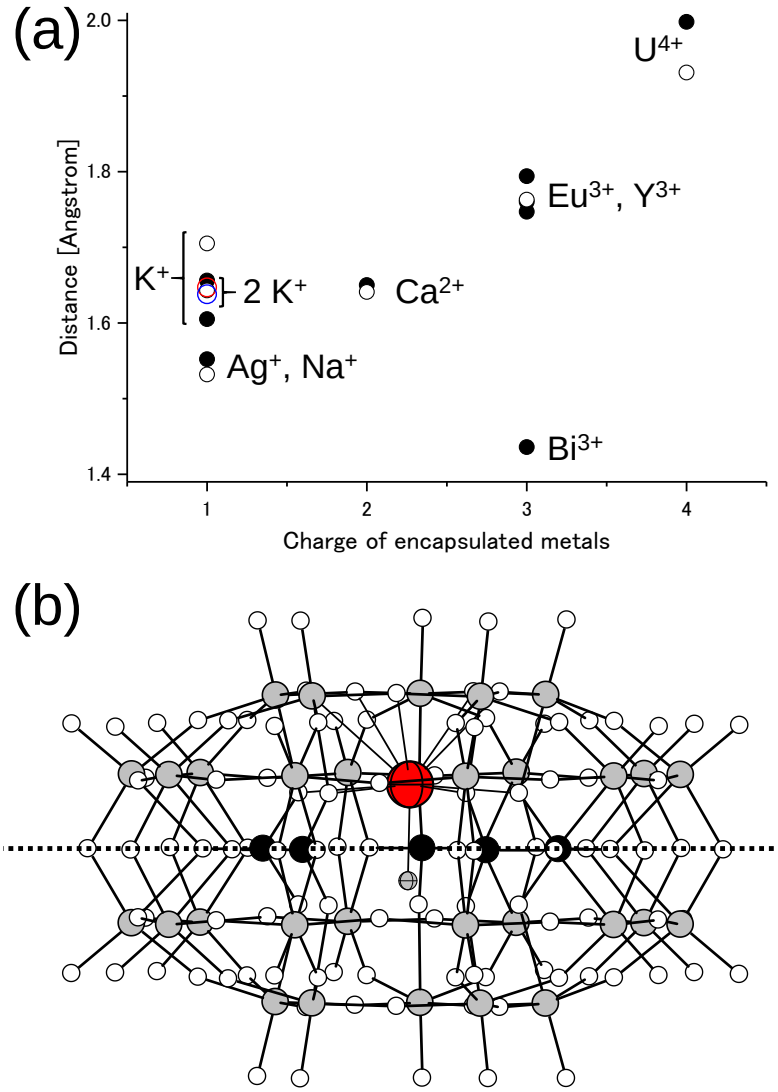


Figure S1. (a) Distances between encapsulated cations and equatorial plane vs. charge of encapsulated cations, red and blue circles, respectively, indicate distance for **1a** and **1c**, and (b) ball-and-stick representation of mono-cation-encapsulated Preyssler-type phosphotungstate. Grey balls, white balls, red ball with a cross line, black balls, and grey ball with cross line indicate W, O, encapsulated cation, P, W, and O (water) atoms, respectively. Dot line indicates equatorial plane of the Preyssler ion through five phosphorous. Data are listed in Table S1.

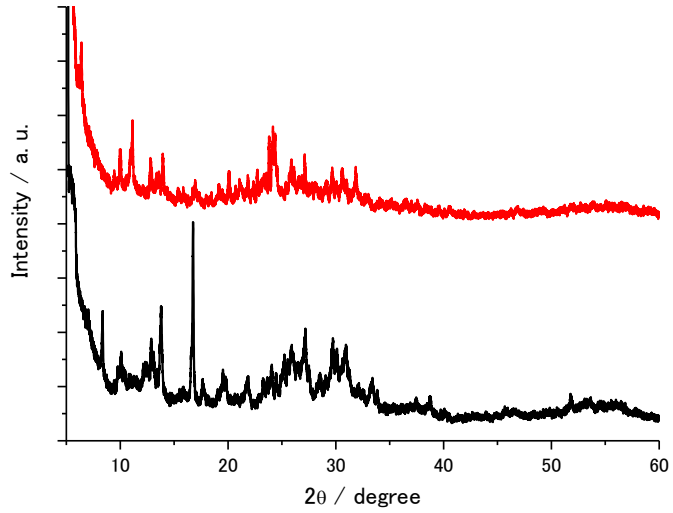
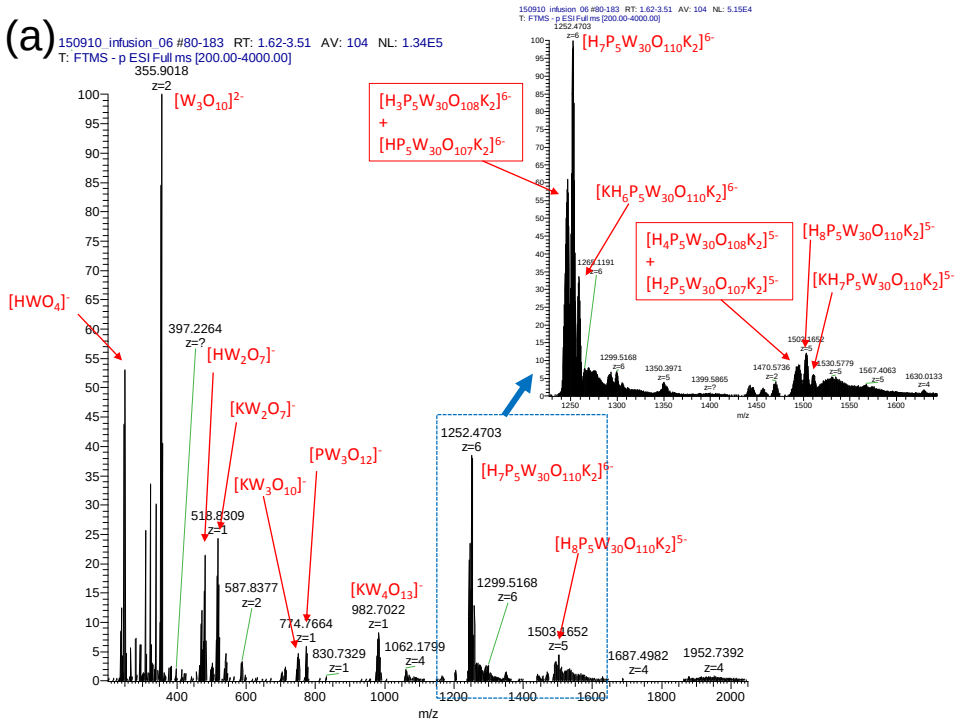
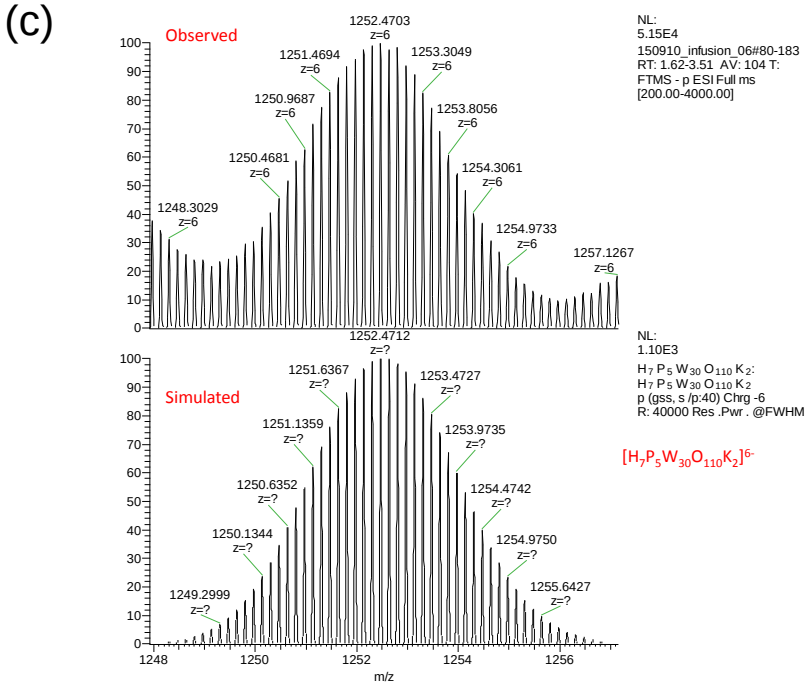
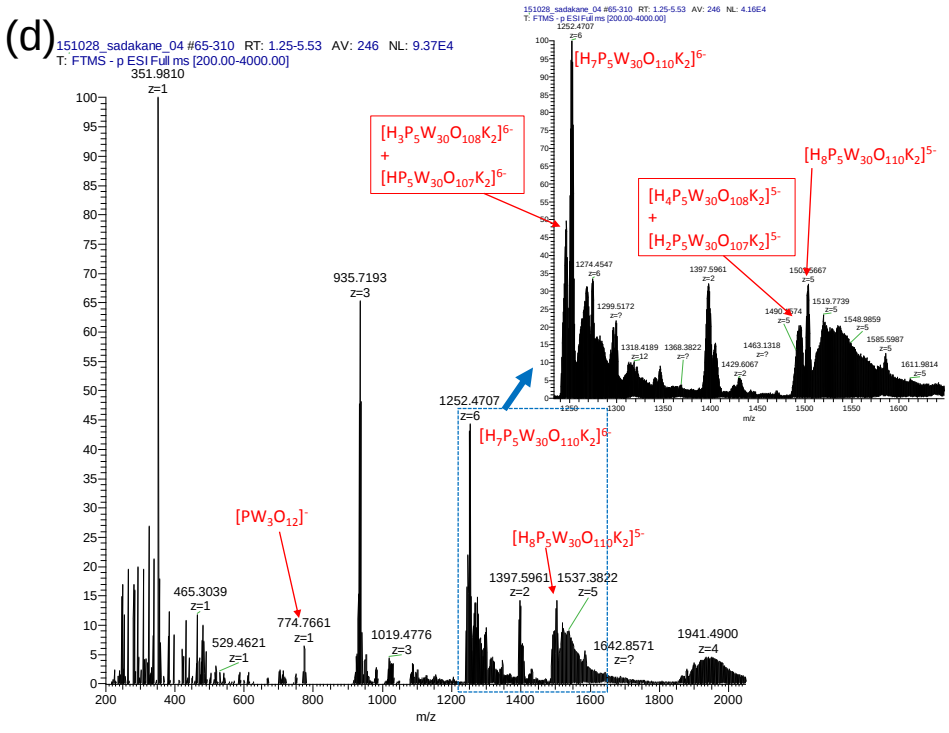


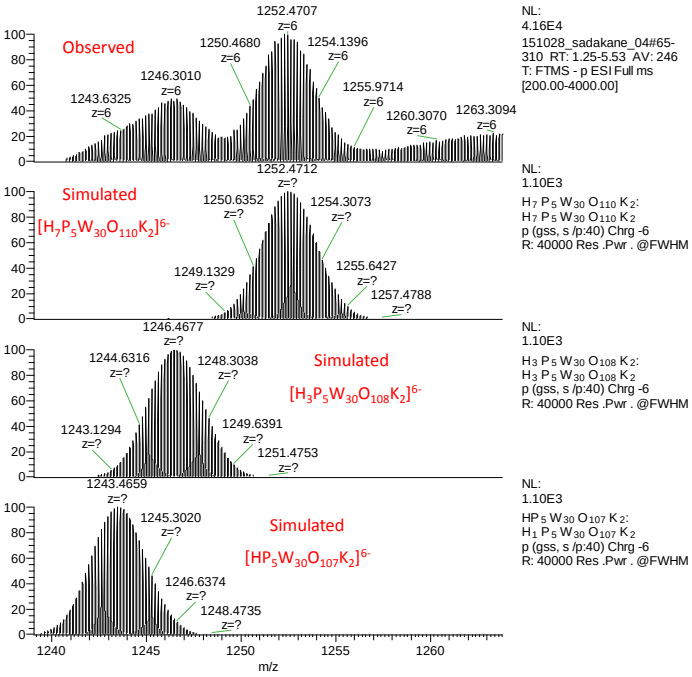
Figure S2. Powder XRD patters of (black line) **1a** and (red line) **1c**. Powder X-ray diffraction (XRD) patterns were obtained on D8 (Brucker) with Cu Kα radiation (tube voltage: 40 kV, tube current: 40 mA).


(a)
150910_infusion_06 #80-183 RT: 1.62-3.51 AV: 104 NL: 1.34E5
T: FTMS - p ESI Full ms [200.00-4000.00]
355.9018
z=2
[W3O10]2-
[HWO4]-
397.2264
z=?
[HW2O7]-
[KW2O7]-
[PW3O12]-
[KW3O10]-
518.8309
z=1
587.8377
z=2
774.7664
z=1
830.7329
z=1
[KW4O13]-
982.7022
z=1
1062.1799
z=4
1252.4703
z=6
[H7P5W30O110K2]6-
1299.5168
z=6
1503.1652
z=5
[H8P5W30O110K2]5-
1687.4982
z=4
1952.7392
z=4
m/z
[H3P5W30O108K2]6-
+
[HP5W30O107K2]6-
[KH6P5W30O110K2]6-
[H4P5W30O108K2]5-
+
[H2P5W30O107K2]5-
[H8P5W30O110K2]5-
[KH7P5W30O110K2]5-
(b)
Observed
1249.9677
z=6
1252.4703
z=6
1246.6347
z=6
1254.3061
z=6
1244.1334
z=6
1258.7951
z=6
1261.2990
z=6
NL:
5.15E4
150910_infusion_06#80-183
RT: 1.62-3.51 AV: 104 T:
FTMS - p ESI Full ms
[200.00-4000.00]
1252.4712
z=?
Simulated
[H7P5W30O110K2]6-
1250.6352
z=?
1254.4742
z=?
1248.9660
z=?
1256.1434
z=?
1259.6487
z=?
NL:
1.10E3
H7 P5 W30 O110 K2:
H7 P5 W30 O110 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
Simulated
[KH6P5W30O110K2]6-
1258.7972
z=?
1256.9611
z=?
1260.8001
z=?
1255.2920
z=?
NL:
1.09E3
H6 KP5 W30 O110 K2:
H6 K3 P5 W30 O110
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
Simulated
[H3P5W30O108K2]6-
1246.4677
z=?
1244.6316
z=?
1248.4707
z=?
1242.9625
z=?
1250.1399
z=?
1253.6453
z=?
NL:
1.10E3
H3 P5 W30 O108 K2:
H3 P5 W30 O108 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
Simulated
[HP5W30O107K2]6-
1243.4659
z=?
1245.4690
z=?
1247.1381
z=?
1250.4764
z=?
NL:
1.10E3
HP5 W30 O107 K2:
H1 P5 W30 O107 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
m/z

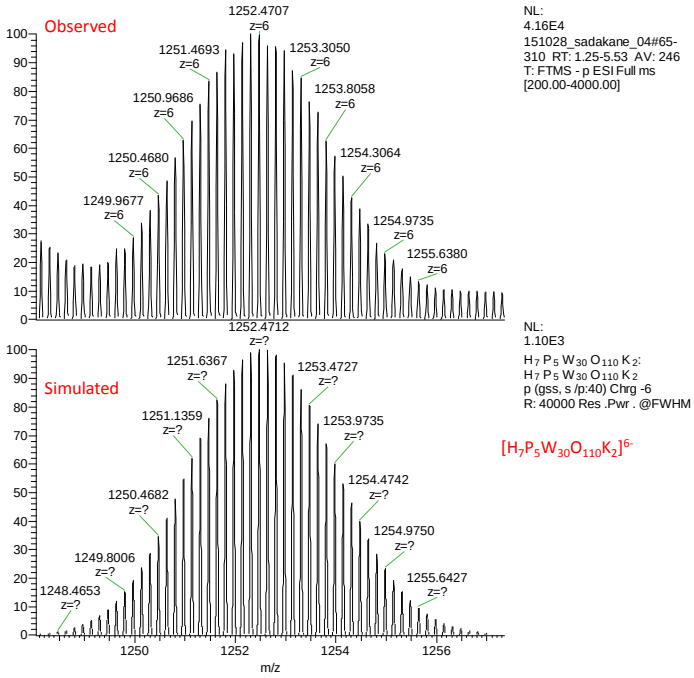

(c)
Observed
1252.4703 z=6
1251.4694 z=6
1253.3049 z=6
1250.9687 z=6
1253.8056 z=6
1250.4681 z=6
1254.3061 z=6
1248.3029 z=6
1254.9733 z=6
1257.1267 z=6
NL: 5.15E4
150910_infusion_06#80-183 RT: 1.62-3.51 AV: 104 T: FTMS - p ESI Full ms [200.00-4000.00]
Simulated
1252.4712 z=?
1251.6367 z=?
1253.4727 z=?
1251.1359 z=?
1253.9735 z=?
1250.6352 z=?
1254.4742 z=?
1250.1344 z=?
1254.9750 z=?
1249.2999 z=?
1255.6427 z=?
NL: 1.10E3
H7 P5 W30 O110 K2:
H7 P5 W30 O110 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
[H7P5W30O110K2]6-
m/z


(d)
151028_sadakane_04 #65-310 RT: 1.25-5.53 AV: 246 NL: 9.37E4
T: FTMS - p ESI Full ms [200.00-4000.00]
351.9810 z=1
935.7193 z=3
[H7P5W30O110K2]6-
[H3P5W30O108K2]6- + [HP5W30O107K2]6-
[H4P5W30O108K2]5- + [H2P5W30O107K2]5-
[H8P5W30O110K2]5-
1252.4707 z=6
[PW3O12]-
465.3039 z=1
529.4621 z=1
774.7661 z=1
1019.4776 z=3
1397.5961 z=2
1537.3822 z=5
1642.8571 z=?
1941.4900 z=4
m/z

(e)


Observed
1252.4707 z=6
1250.4680 z=6
1254.1396 z=6
1246.3010 z=6
1243.6325 z=6
1255.9714 z=6
1260.3070 z=6
1263.3094 z=6
NL: 4.16E4
151028_sadakane_04#65-310 RT: 1.25-5.53 AV: 246
T: FTMS - p ESI Full ms [200.00-4000.00]
Simulated
[H7P5W30O110K2]6-
1252.4712 z=?
1250.6352 z=?
1254.3073 z=?
1249.1329 z=?
1255.6427 z=?
1257.4788 z=?
NL: 1.10E3
H7 P5 W30 O110 K2: H7 P5 W30 O110 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
Simulated
[H3P5W30O108K2]6-
1246.4677 z=?
1244.6316 z=?
1248.3038 z=?
1243.1294 z=?
1249.6391 z=?
1251.4753 z=?
NL: 1.10E3
H3 P5 W30 O108 K2: H3 P5 W30 O108 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
Simulated
[HP5W30O107K2]6-
1243.4659 z=?
1245.3020 z=?
1246.6374 z=?
1248.4735 z=?
NL: 1.10E3
HP5 W30 O107 K2: H1 P5 W30 O107 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
m/z

(f)


Observed
1252.4707 z=6
1251.4693 z=6
1253.3050 z=6
1250.9686 z=6
1253.8058 z=6
1250.4680 z=6
1254.3064 z=6
1249.9677 z=6
1254.9735 z=6
1255.6380 z=6
NL: 4.16E4
151028_sadakane_04#65-310 RT: 1.25-5.53 AV: 246
T: FTMS - p ESI Full ms [200.00-4000.00]
Simulated
1252.4712 z=?
1251.6367 z=?
1253.4727 z=?
1251.1359 z=?
1253.9735 z=?
1254.4742 z=?
1250.4682 z=?
1254.9750 z=?
1249.8006 z=?
1255.6427 z=?
1248.4653 z=?
NL: 1.10E3
H7 P5 W30 O110 K2: H7 P5 W30 O110 K2
p (gss, s /p:40) Chrg -6
R: 40000 Res .Pwr . @FWHM
[H7P5W30O110K2]6-
m/z

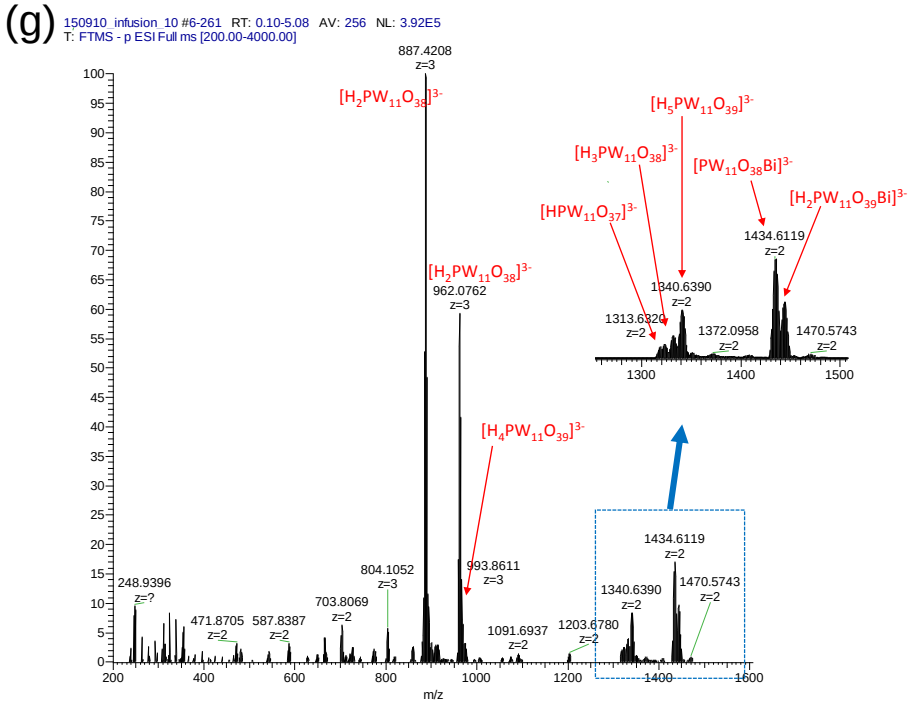


Figure S3. ESI-MS of (a), (b), and (c) **1a**, (d), (e), and (f) **1b**, and (g) solid isolated from the reaction solution.

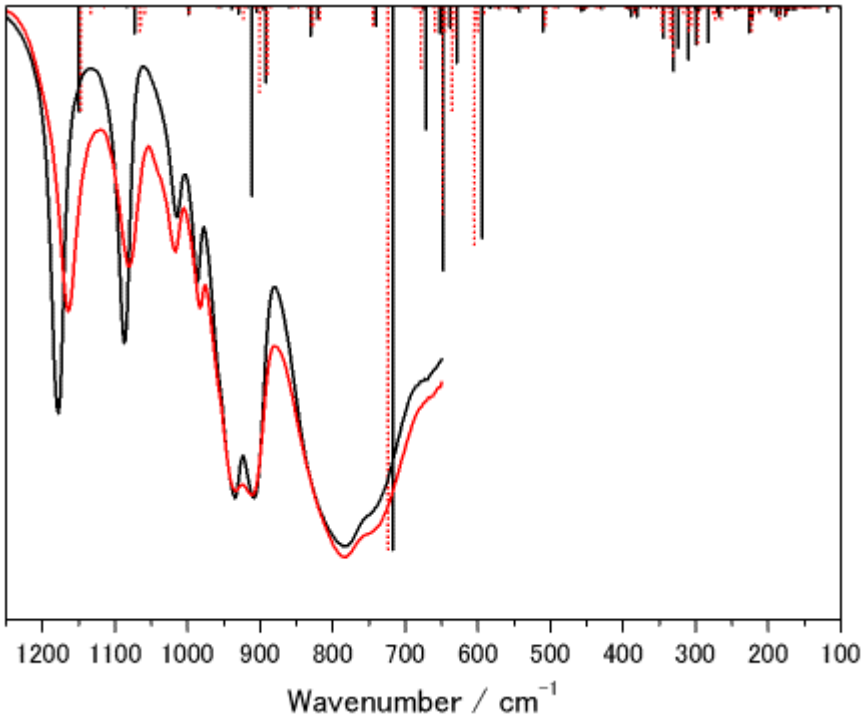


Figure S4. Computed IR spectra for (black bars) $[P_5W_{30}O_{110}K_2]$ and (red bars) $[P_5W_{30}O_{110}Na(H_2O)]$ structures and observed IR spectra for (black line) $K_{13}[P_5W_{30}O_{110}K_2]$ (**1a**) and (red line) $K_{14}[P_5W_{30}O_{110}Na]$.

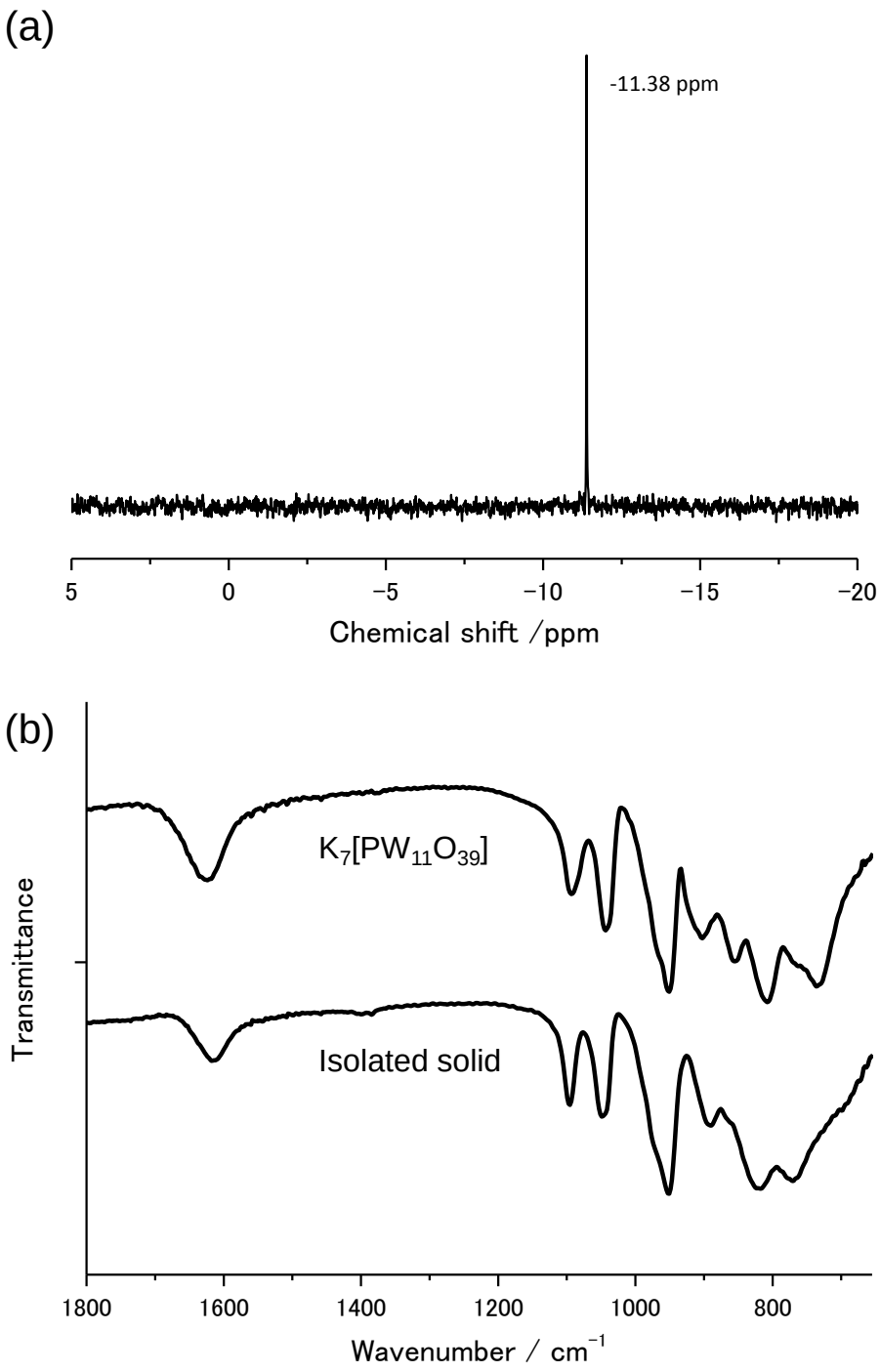


Figure S5. (a) ^{31}P NMR and (b) IR of isolated solid by cooling the filtrate (^{31}P NMR of the filtrate was shown in Figure 2 (a)) in a refrigerator. Sample (50 mg) was dissolved in D_2O (1 ml) for ^{31}P NMR.

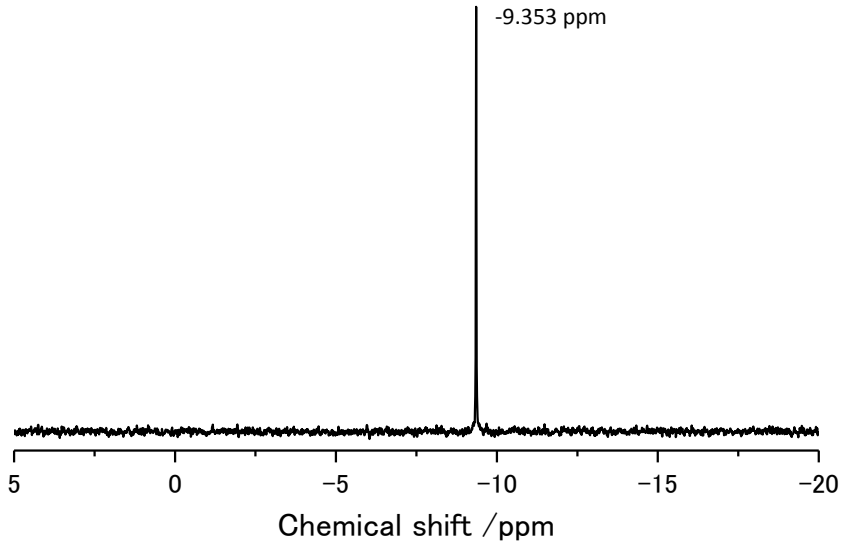


Figure S6. ^{31}P NMR of solution obtained after a reaction of $K_{14}[P_5W_{30}O_{110}Na(H_2O)]$ in KOAc buffer (pH 4.7) in the presence of KCl.

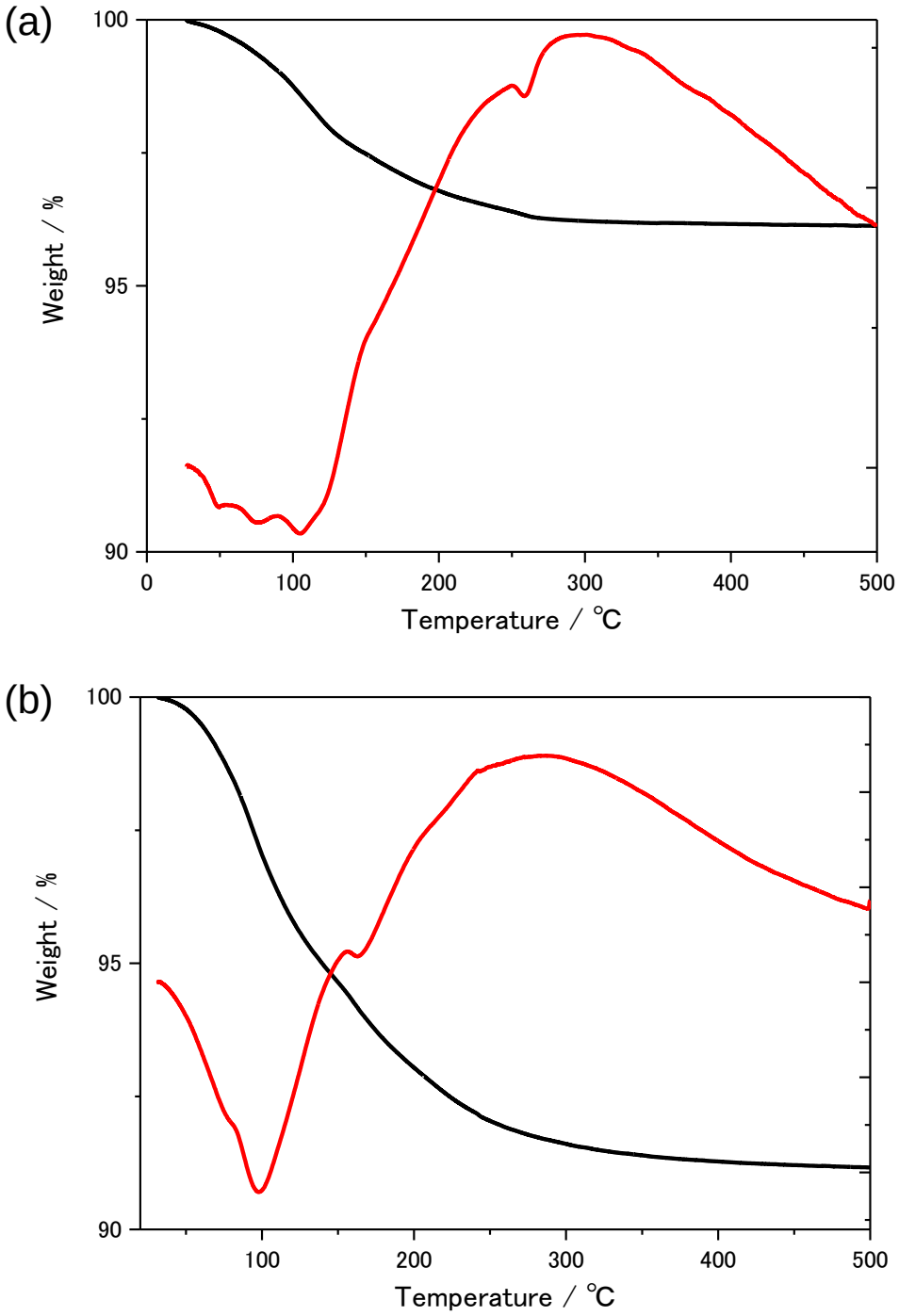


Figure S7. TG-DTA profiles of (a) **1a** and (b) **1b**. Black and red line indicate TG and DTA profiles, respectively. TG-DTA was measured using TG/DTA7300 (SII, Japan) with 10 ºC·min^{-1} of heating rate under N_2 flow of 50 ml·s^{-1}.

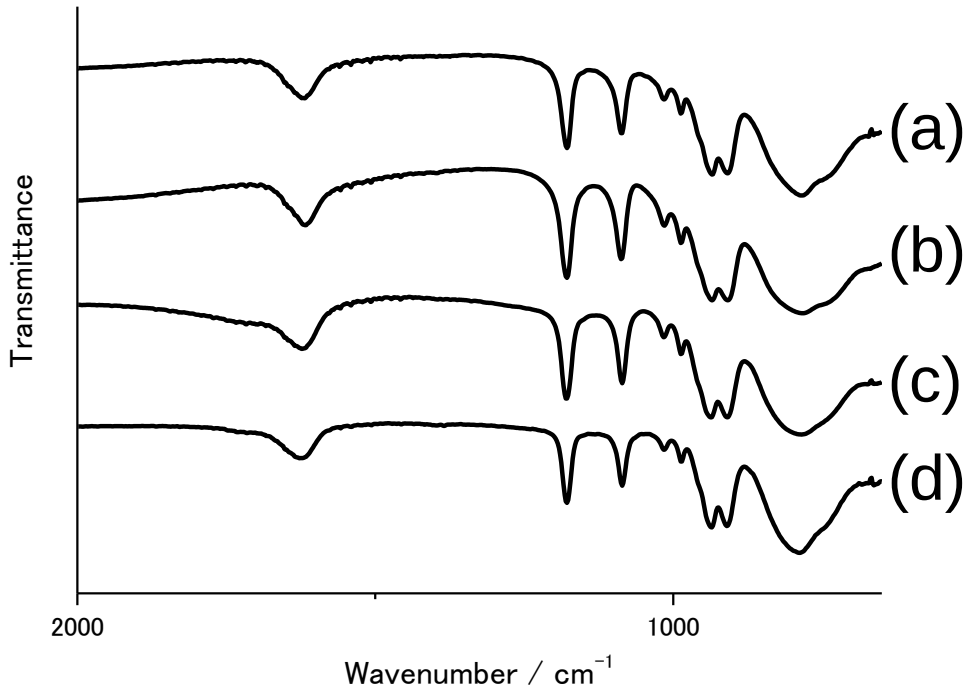


Figure S8. IR of (a) $K_{13}[P_5W_{30}O_{110}K_2]$ (**1a**) after heating at 400 °C, (b) $K_{13}[P_5W_{30}O_{110}K_2]$ (**1a**) without heating, (c) $H_{13}[P_5W_{30}O_{110}K_2]$ (**1b**) without heating, and (d) $H_{13}[P_5W_{30}O_{110}K_2]$ (**1b**) after heating at 100 °C.

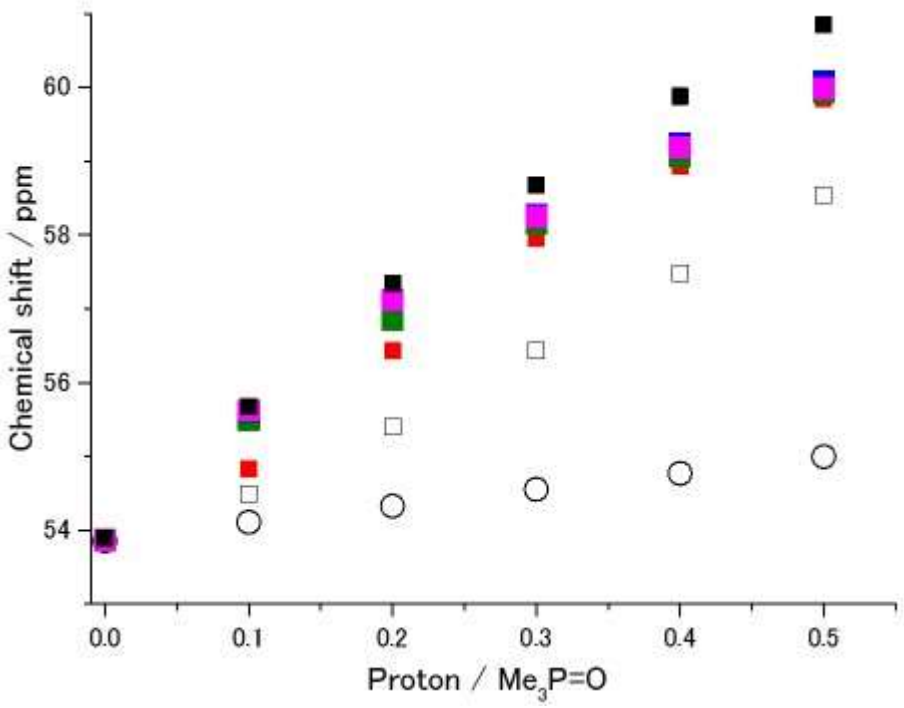


Figure S9. Change in ^{31}P NMR chemical shift of $Me_3P=O$ (1 mM) in D_2O in the presence of (black squares) $H_{13}[P_5W_{30}O_{110}K_2]$, (red squares) $H_{14}[P_5W_{30}O_{110}Na]$, (green squares) $H_{13}[P_5W_{30}O_{110}Ca]$, (pink squares) $H_{12}[P_5W_{30}O_{110}Eu]$, (blue squares) $H_{12}[P_5W_{30}O_{110}Bi]$, (open squares) Keggin-type phosphotungstic acid, and (open balls) sulfuric acid.

Table S1. Selected distances of Preyssler-type phosphotungstates with different encapsulated matels.

No.	Preyssler compounds	Encaps. metal	Distances [Å][a]			Ref.
			M-O(P)	$M-O_b$	M-plane[b]	
1	$(NH_4)_{14}[P_5W_{30}O_{110}Na(H_2O)]$	mono-Na^+	2.64	2.99	1.552	[1]
2	$Ag_{19}(ptz)_8(H_2ptz)(H_3ptz)$ -$[P_5W_{30}O_{110}Ag(H_2O)]$[c]	mono-Ag^+	2.65	3.00	1.532	[2]
3	$Co_4(dimb)_4(H_2O)_8H_6$ -$[P_5W_{30}O_{110}K(H_2O)]$[d]	mono-K^+	2.71	3.03	1.656	[3]
4	$Co_4(dimb)_4(H_2O)_8H_6$ -$[P_5W_{30}O_{110}K(H_2O)]$[d]	mono-K^+	2.66	2.95	1.634	[3]
5	$Cu_{10}(ttbz)_2(Httbz)_4(OH)_6(H_2O)_8$ -$[P_5W_{30}O_{110}K(H_2O)]$[e]	mono-K^+	2.66	2.99	1.605	[4]
6	$Co_4(bpz)_2(H_2O)_9$ -$[P_5W_{30}O_{110}K(H_2O)]$[f]	mono-K^+	2.65	2.83	1.705	[4]
7	$K_{13}[P_5W_{30}O_{110}K_2]$ (**1a**)	di-K^+	2.71	2.90	1.638	This work
8	$H_{13}[P_5W_{30}O_{110}K_2]$ (**1b**)	di-K^+	2.71	2.92	1.647	This work
9	$(NH_4)_{13}[P_5W_{30}O_{110}Ca]$	mono-Ca^{2+}	2.68	2.90	1.650	[1]
10	$K_5H_8[P_5W_{30}O_{110}Ca]$	mono-Ca^{2+}	2.62	2.89	1.641	[1]
11	$K_{12}[P_5W_{30}O_{110}Bi]$	mono-Bi^{3+}	2.58	3.05	1.436	[5]
12	$(NH_4)_{12}[P_5W_{30}O_{110}Y]$	mono-Y^{3+}	2.60	2.73	1.747	[1]
13	$K_5H_7[P_5W_{30}O_{110}Y]$	mono-Y^{3+}	2.61	2.78	1.794	[1]
14	$K_{0.5}(NH_4)_{11.5}[P_5W_{30}O_{110}Eu]$	mono-Eu^{3+}	2.62	2.75	1.763	[6]
15	$K_6H_6[P_5W_{30}O_{110}Eu]$	mono-Eu^{3+}	2.62	2.82	1.760	[6]
16	$(NH_4)_{11}[P_5W_{30}O_{110}U]$	mono-U^{4+}	2.65	2.59	1.931	[6]
17	$K_3H_8[P_5W_{30}O_{110}U]$	mono-U^{4+}	2.66	2.67	1.998	[6]

[a] mean distances. [b] distance between encapsulated cation (M) and equatorial plane through five phosphorous. [c] Hptz: 5-phenyl-1H-tetrazole. [d] dimb: 1,3-di(1H-imidazol-1-yl)benzene. [e] Httbz: 1-(tetrazo-5-yl)-4-(triazo-1-yl)benzene. [f] bpz: 3,3',5,5'-tetramethyl-4,4'-bipyrazole.

[1] Kim, K.-C.; Pope, M. T.; Gama, G. J.; Dickman, M. H. Slow Proton Exchange in Aqueous Solution. Consequences of Protonation and Hydration within the Central Cavity of Preyssler Anion Derivatives, $[|M(H_2O)|)P_5W_{30}O_{110}]^{n-}$, *J. Am. Chem. Soc*., **1999**, *121*, 11164-11170.

[2] Liang, M.-X.; Ruan, C.-Z.; Sun, D.; Kong, X.-J.; Ren, Y.-P.; Long, L.-S.; Huang, R.-B.; Zheng, L.-S. Solvothermal Synthesis of Four Polyoxometalate-Based Coordination Polymers Including Diverse Ag(I)···π Interaction, *Inorg. Chem*. **2014**, *53*, 897-902.

[3] Zhao, Y.-Q.; Yu, K.; Wang, L.-W.; Wang, Y.; Wang, X.-P.; Sun, D. Anion-Induced

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[4] Hu, T.-P.; Zhao, Y.-Q.; Jaglicic, Z.; Yu, K.; Wang, X.-P.; Sun, D. Four Hybrid Materials Based on Preyssler P_5W_{30} Polymetalate and First-Row Transition-Metal Complex, *Inorg. Chem*. **2015**, *54*, 7415-7423.

[5] Hayashi, A.; Haioka, T.; Takahashi, K.; Bassil, B. S.; Kortz, U.; Sano, T.; Sadakane, M. Cation effect on formation of Preyssler-type 30-tungsto-5-phosphate: enhanced yield of Na-encapsulated derivative and direct synthesis of Ca- and Bi-encapsulated derivatives, *Z. anorg. allg. Chem*. **2015**, *641*, 2670-2676.

[6] Dickman, M, H.; Gama, G. J.; Kim, K.-C.; Pope, M. T. The Structure of Europium(III)- and Uranium(IV) Derivatives of $[P_5W_{30}O_{110}]^{15-}$: Evidence for "Cryptohydration", *J. Cluster Sci*. **1996**, *7*, 567-583.

Table S2. DFT optimized structures for $[P_5W_{30}O_{110}K_2]$ and $[P_5W_{30}O_{110}Na(H_2O)]$ compounds (see electronic structure details). Cartesian coordinates in Ångstrom.

$[P_5W_{30}O_{110}K_2]$

K	0.000000	0.000000	1.584645
K	0.000000	0.000000	-1.584645
P	-3.617288	0.000000	0.000000
W	-6.021680	-1.721043	1.684783
W	-5.828263	2.086177	1.671684
W	-0.223992	-6.258790	1.684783
W	-3.785104	-4.898344	1.671684
W	5.883246	-2.147102	1.684783
W	3.488940	-5.113519	1.671684
W	3.860038	4.931808	1.684783
W	5.941388	1.738015	1.671684
W	-3.497611	5.195127	1.684783
W	0.183039	6.187672	1.671684
W	-6.021680	1.721043	-1.684783
W	-5.828263	-2.086177	-1.671684
W	-0.223992	6.258790	-1.684783
W	-3.785104	4.898344	-1.671684
W	5.883246	2.147102	-1.684783
W	3.488940	5.113519	-1.671684
W	3.860038	-4.931808	-1.684783
W	5.941388	-1.738015	-1.671684
W	-3.497611	-5.195127	-1.684783
W	0.183039	-6.187672	-1.671684
W	-3.247678	-0.020837	3.396322
O	-2.760500	-0.003130	1.258911
O	-4.542139	-1.264152	-0.001783
O	-4.542139	1.264152	0.001783
O	-6.481308	0.029098	1.605483
O	-4.564108	1.301868	2.850487
O	-4.576987	-1.319676	2.864198
O	-6.815106	-2.263246	-0.002269
O	-6.815106	2.263246	0.002269
O	-1.900009	-1.389102	3.479812

O	-5.039732	-3.601089	1.587368
O	-3.670633	-0.008366	5.087722
O	-7.240875	-2.338807	2.769365
O	-7.140644	2.459555	2.758862
P	-1.117803	-3.440245	0.000000
W	-0.983771	-3.095165	3.396322
O	-0.850065	-2.626359	1.258911
O	-0.201318	-4.710476	-0.001783
O	-2.605878	-3.929187	0.001783
O	-2.030508	-6.155099	1.605483
O	-2.648536	-3.938425	2.850487
O	-0.159280	-4.760776	2.864198
O	0.046491	-7.180933	-0.002269
O	-4.258459	-5.782170	0.002269
O	0.733979	-2.236272	3.479812
O	1.867477	-5.905868	1.587368
O	-1.126331	-3.493564	5.087722
O	-0.013215	-7.609213	2.769365
O	-4.545756	-6.031111	2.758862
P	2.926447	-2.126189	0.000000
W	2.639675	-1.892080	3.396322
O	2.235131	-1.620049	1.258911
O	4.417718	-1.647082	-0.001783
O	2.931618	-3.692523	0.001783
O	5.226385	-3.833158	1.605483
O	2.927222	-3.735948	2.850487
O	4.478547	-1.622645	2.864198
O	6.843840	-2.174814	-0.002269
O	4.183234	-5.836824	0.002269
O	2.353633	0.007010	3.479812
O	6.193896	-0.048938	1.587368
O	2.974521	-2.150776	5.087722
O	7.232708	-2.363945	2.769365
O	4.331212	-6.186987	2.758862
P	2.926447	2.126189	0.000000
W	2.615179	1.925795	3.396322

O	2.231452	1.625113	1.258911
O	2.931618	3.692523	-0.001783
O	4.417718	1.647082	0.001783
O	5.260592	3.786077	1.605483
O	4.457659	1.629482	2.850487
O	2.927175	3.757926	2.864198
O	4.183234	5.836824	-0.002269
O	6.843840	2.174814	0.002269
O	0.720646	2.240604	3.479812
O	1.960562	5.875623	1.587368
O	2.964687	2.164312	5.087722
O	4.483275	6.148215	2.769365
O	7.222593	2.207343	2.758862
P	-1.117803	3.440245	0.000000
W	-1.023405	3.082287	3.396322
O	-0.856018	2.624424	1.258911
O	-2.605878	3.929187	-0.001783
O	-0.201318	4.710476	0.001783
O	-1.975161	6.173082	1.605483
O	-0.172237	4.743024	2.850487
O	-2.669453	3.945171	2.864198
O	-4.258459	5.782170	-0.002269
O	0.046491	7.180933	0.002269
O	-1.908249	1.377760	3.479812
O	-4.982202	3.680272	1.587368
O	-1.142244	3.488394	5.087722
O	-4.461892	6.163751	2.769365
O	0.132596	7.551200	2.758862
W	-3.247678	0.020837	-3.396322
O	-2.760500	0.003130	-1.258911
O	-6.481308	-0.029098	-1.605483
O	-4.564108	-1.301868	-2.850487
O	-4.576987	1.319676	-2.864198
O	-1.900009	1.389102	-3.479812
O	-5.039732	3.601089	-1.587368
O	-3.670633	0.008366	-5.087722

O	-7.240875	2.338807	-2.769365
O	-7.140644	-2.459555	-2.758862
W	-0.983771	3.095165	-3.396322
O	-0.850065	2.626359	-1.258911
O	-2.030508	6.155099	-1.605483
O	-2.648536	3.938425	-2.850487
O	-0.159280	4.760776	-2.864198
O	0.733979	2.236272	-3.479812
O	1.867477	5.905868	-1.587368
O	-1.126331	3.493564	-5.087722
O	-0.013215	7.609213	-2.769365
O	-4.545756	6.031111	-2.758862
W	2.639675	1.892080	-3.396322
O	2.235131	1.620049	-1.258911
O	5.226385	3.833158	-1.605483
O	2.927222	3.735948	-2.850487
O	4.478547	1.622645	-2.864198
O	2.353633	-0.007010	-3.479812
O	6.193896	0.048938	-1.587368
O	2.974521	2.150776	-5.087722
O	7.232708	2.363945	-2.769365
O	4.331212	6.186987	-2.758862
W	2.615179	-1.925795	-3.396322
O	2.231452	-1.625113	-1.258911
O	5.260592	-3.786077	-1.605483
O	4.457659	-1.629482	-2.850487
O	2.927175	-3.757926	-2.864198
O	0.720646	-2.240604	-3.479812
O	1.960562	-5.875623	-1.587368
O	2.964687	-2.164312	-5.087722
O	4.483275	-6.148215	-2.769365
O	7.222593	-2.207343	-2.758862
W	-1.023405	-3.082287	-3.396322
O	-0.856018	-2.624424	-1.258911
O	-1.975161	-6.173082	-1.605483
O	-0.172237	-4.743024	-2.850487

O	-2.669453	-3.945171	-2.864198
O	-1.908249	-1.377760	-3.479812
O	-4.982202	-3.680272	-1.587368
O	-1.142244	-3.488394	-5.087722
O	-4.461892	-6.163751	-2.769365
O	0.132596	-7.551200	-2.758862

$[P_5W_{30}O_{110}Na(H_2O)]$

Na	0.081118	-0.005899	1.412836
O	0.021079	0.002129	-0.891745
H	-0.497118	0.775575	-1.138040
H	-0.511117	-0.759647	-1.142865
P	-3.634536	-0.000054	0.000367
W	-6.035094	-1.718085	1.685569
W	-5.836539	2.095014	1.671017
W	-0.230884	-6.262695	1.689716
W	-3.792313	-4.894860	1.677362
W	5.898152	-2.161001	1.687451
W	3.488319	-5.126986	1.674893
W	3.874940	4.938205	1.689198
W	5.957035	1.732950	1.673941
W	-3.495608	5.201086	1.690480
W	0.187969	6.190637	1.676226
W	-6.031492	1.716256	-1.683964
W	-5.835549	-2.092457	-1.668690
W	-0.229602	6.260486	-1.678136
W	-3.792860	4.901291	-1.664582
W	5.884342	2.160594	-1.679941
W	3.487369	5.122326	-1.664484
W	3.876382	-4.931895	-1.679435
W	5.948462	-1.730634	-1.665762
W	-3.500317	-5.204432	-1.678399
W	0.187212	-6.191209	-1.664498
W	-3.239067	-0.021032	3.363996
O	-2.756666	-0.011627	1.242536
O	-4.559925	-1.266339	0.004325

O	-4.560895	1.265248	0.014885
O	-6.501540	0.028457	1.613703
O	-4.563006	1.303392	2.834872
O	-4.578853	-1.322791	2.850675
O	-6.832801	-2.264581	0.004722
O	-6.829607	2.268508	0.010140
O	-1.890349	-1.381154	3.452925
O	-5.053400	-3.607122	1.590549
O	-3.660164	-0.009726	5.060150
O	-7.246783	-2.345010	2.777984
O	-7.146676	2.458466	2.769344
P	-1.125177	-3.443999	0.002074
W	-0.974623	-3.076698	3.370008
O	-0.843312	-2.616788	1.246898
O	-0.205597	-4.713273	-0.000652
O	-2.613124	-3.937633	0.015563
O	-2.035767	-6.166700	1.612924
O	-2.647957	-3.931663	2.840301
O	-0.157270	-4.757089	2.852257
O	0.040925	-7.189215	0.007300
O	-4.266130	-5.789292	0.014275
O	0.733416	-2.221077	3.449561
O	1.869220	-5.919820	1.594279
O	-1.115162	-3.475061	5.065780
O	-0.014910	-7.608669	2.782504
O	-4.544124	-6.029149	2.774270
P	2.943838	-2.139426	0.001795
W	2.640841	-1.884688	3.366660
O	2.239535	-1.615483	1.243500
O	4.436916	-1.656759	0.010347
O	2.953550	-3.708906	0.023572
O	5.246805	-3.846688	1.623035
O	2.926733	-3.735448	2.841368
O	4.484351	-1.620663	2.855094
O	6.861279	-2.183792	0.011844
O	4.190072	-5.853859	0.018220

O	2.340192	0.008500	3.442615
O	6.214019	-0.050038	1.595796
O	2.964293	-2.134524	5.065701
O	7.245302	-2.362261	2.782855
O	4.332530	-6.191311	2.775259
P	2.941263	2.140428	0.003601
W	2.613933	1.921756	3.367573
O	2.223995	1.632943	1.245011
O	2.947714	3.709927	0.015607
O	4.435083	1.660581	0.022968
O	5.279567	3.801661	1.624100
O	4.458592	1.627306	2.841286
O	2.927407	3.761216	2.857792
O	4.195102	5.851502	0.012754
O	6.859630	2.180582	0.018397
O	0.717196	2.228710	3.452348
O	1.963471	5.887860	1.592203
O	2.951296	2.151073	5.066891
O	4.479321	6.160189	2.783933
O	7.227739	2.209721	2.775598
P	-1.124581	3.442229	0.003884
W	-1.016128	3.064708	3.370789
O	-0.863535	2.609351	1.249342
O	-2.612847	3.935794	0.006778
O	-0.205290	4.711759	0.010154
O	-1.980328	6.186086	1.613654
O	-0.171710	4.737680	2.839684
O	-2.671645	3.941172	2.854087
O	-4.262886	5.792514	0.006715
O	0.042614	7.187471	0.012992
O	-1.901176	1.368627	3.453596
O	-4.996919	3.689769	1.590430
O	-1.138604	3.469245	5.066606
O	-4.465629	6.162247	2.781239
O	0.130674	7.549232	2.773644
W	-3.234058	0.020088	-3.368886

O	-2.823560	0.013255	-1.284627
O	-6.508209	-0.026793	-1.596607
O	-4.584932	-1.305812	-2.841115
O	-4.599190	1.326210	-2.859107
O	-1.917750	1.401852	-3.487336
O	-5.049564	3.609506	-1.572785
O	-3.703725	0.009256	-5.054509
O	-7.254086	2.349463	-2.760539
O	-7.155414	-2.466017	-2.751925
W	-0.985096	3.085684	-3.378023
O	-0.868109	2.652794	-1.272902
O	-2.035584	6.170504	-1.594573
O	-2.656938	3.951106	-2.839066
O	-0.161259	4.770938	-2.852031
O	0.736520	2.261888	-3.489117
O	1.869670	5.920724	-1.567948
O	-1.142444	3.519780	-5.064038
O	-0.011061	7.615258	-2.760003
O	-4.555229	6.038953	-2.750354
W	2.613503	1.875850	-3.346201
O	2.300491	1.666546	-1.285622
O	5.250163	3.852532	-1.587165
O	2.941579	3.756922	-2.834455
O	4.501580	1.631314	-2.847624
O	2.377747	-0.009988	-3.481435
O	6.215081	0.049983	-1.564773
O	3.002419	2.170051	-5.030072
O	7.248153	2.367456	-2.754799
O	4.335845	6.205106	-2.743974
W	2.589370	-1.914007	-3.347281
O	2.285537	-1.688284	-1.286891
O	5.288597	-3.808307	-1.588688
O	4.479216	-1.638017	-2.833238
O	2.945500	-3.782843	-2.852383
O	0.720414	-2.270334	-3.488763
O	1.961111	-5.891421	-1.570638

O	2.988420	-2.184906	-5.032840
O	4.490883	-6.168866	-2.752078
O	7.238546	-2.206896	-2.746361
W	-1.025588	-3.075283	-3.378329
O	-0.891093	-2.648510	-1.275025
O	-1.987363	-6.191863	-1.592764
O	-0.178992	-4.754268	-2.836853
O	-2.683311	-3.960273	-2.855963
O	-1.927793	-1.390342	-3.486971
O	-4.997891	-3.688058	-1.573332
O	-1.157559	-3.514995	-5.065280
O	-4.476453	-6.173362	-2.756356
O	0.130732	-7.558757	-2.751415

Table S3. List of computed frequencies and intensities

K2_Preyssler compound

Frequency (degeneracy not counted)	Dipole Strength	Absorption Intensity
cm-1	1e-40 esu2 cm2	km/mole
29.417440	0.000000	0.000000
29.417440	0.000000	0.000000
32.791789	0.000000	0.000000
33.356463	1.734320	0.014501
33.356463	1.734320	0.014501
44.129845	0.000000	0.000000
44.129845	0.000000	0.000000
48.601276	9.644128	0.117487
49.854264	146.879918	1.835451
49.854264	146.879918	1.835451
56.375056	0.000078	0.000001
58.403098	0.000000	0.000000
58.403098	0.000000	0.000000
62.524902	153.876038	2.411582
65.653886	265.766930	4.373604
65.653886	265.766930	4.373604
67.733139	0.000000	0.000000
67.733139	0.000000	0.000000
72.222952	0.000101	0.000002
74.294379	1038.550532	19.340231
74.294379	1038.550532	19.340231
75.369418	44.042487	0.832042
77.648152	173.535775	3.377522
77.648152	173.535775	3.377522
79.755665	0.000000	0.000000
79.755665	0.000000	0.000000
83.168206	0.000007	0.000000
85.656013	3201.373184	68.734097
85.656013	3201.373184	68.734097

86.300963	0.000000	0.000000
86.300963	0.000000	0.000000
88.176579	1690.009433	37.352566
92.775388	0.000000	0.000000
92.775388	0.000000	0.000000
94.449154	0.000000	0.000000
94.449154	0.000000	0.000000
94.522386	157.484789	3.731224
94.522386	157.484789	3.731224
100.440872	1017.618069	25.619660
100.440872	1017.618069	25.619660
102.540900	0.000607	0.000016
106.187087	0.000000	0.000000
106.187087	0.000000	0.000000
106.720843	0.000000	0.000000
106.720843	0.000000	0.000000
115.000531	0.000957	0.000028
117.327071	0.000000	0.000000
117.327071	0.000000	0.000000
117.962931	8446.732801	249.753958
117.962931	8446.732801	249.753958
123.354431	0.000000	0.000000
123.354431	0.000000	0.000000
128.411441	76.755552	2.470538
129.773470	0.000021	0.000001
131.314473	0.000000	0.000000
131.314473	0.000000	0.000000
131.348585	737.189870	24.270729
131.348585	737.189870	24.270729
135.587601	0.000000	0.000000
135.587601	0.000000	0.000000
139.514531	95.249605	3.330893
139.514531	95.249605	3.330893
140.117891	0.000049	0.000002
140.817097	119.751748	4.226835
140.817097	119.751748	4.226835

140.838832	0.000000	0.000000
140.838832	0.000000	0.000000
142.352249	1810.771743	64.610948
142.352249	1810.771743	64.610948
145.856404	86.155645	3.149831
146.338764	0.000000	0.000000
146.338764	0.000000	0.000000
146.777067	117.643256	4.328160
146.777067	117.643256	4.328160
147.859769	0.000001	0.000000
147.980773	1184.468275	43.934612
147.980773	1184.468275	43.934612
148.563515	342.010005	12.735883
150.668678	2028.592953	76.611852
150.668678	2028.592953	76.611852
152.209436	0.000000	0.000000
152.209436	0.000000	0.000000
152.659165	441.446588	16.891924
152.659165	441.446588	16.891924
155.679545	135.149360	5.273800
159.848328	0.000003	0.000000
160.058565	0.000000	0.000000
160.058565	0.000000	0.000000
162.203569	3658.240677	148.734168
162.203569	3658.240677	148.734168
165.203346	0.000006	0.000000
167.140672	3834.265908	160.635838
167.140672	3834.265908	160.635838
167.173344	0.000000	0.000000
167.173344	0.000000	0.000000
171.076157	266.704064	11.436607
172.610371	3903.536581	168.889717
172.610371	3903.536581	168.889717
173.066335	0.000000	0.000000
173.066335	0.000000	0.000000
176.400753	0.000000	0.000000

176.400753	0.000000	0.000000
176.827810	10163.469448	450.474929
176.827810	10163.469448	450.474929
177.509210	14.432065	0.642137
177.509210	14.432065	0.642137
178.397689	1110.962090	49.678278
179.213299	0.000000	0.000000
179.719327	0.000000	0.000000
179.719327	0.000000	0.000000
183.004403	309.230168	14.184743
183.713105	0.000008	0.000000
183.828253	9162.336229	422.178931
183.828253	9162.336229	422.178931
184.464762	0.000000	0.000000
184.464762	0.000000	0.000000
186.053530	847.591250	39.527782
186.053530	847.591250	39.527782
188.110409	0.000000	0.000000
188.110409	0.000000	0.000000
188.485782	9924.805786	468.898326
188.485782	9924.805786	468.898326
190.549672	52.410709	2.503262
190.683827	0.000000	0.000000
190.683827	0.000000	0.000000
195.503256	4336.690485	212.515441
195.503256	4336.690485	212.515441
196.455219	0.250072	0.012314
196.836019	0.000000	0.000000
196.836019	0.000000	0.000000
201.298364	0.000000	0.000000
201.298364	0.000000	0.000000
202.319949	260.049935	13.187836
202.319949	260.049935	13.187836
204.014707	0.000003	0.000000
204.257950	0.000000	0.000000
204.257950	0.000000	0.000000

206.798619	0.000000	0.000000
206.798619	0.000000	0.000000
206.859997	1310.933919	67.972835
206.859997	1310.933919	67.972835
206.967019	0.000001	0.000000
209.953538	133.347955	7.017584
212.361286	0.000000	0.000000
212.361286	0.000000	0.000000
212.739097	4988.038597	265.983801
212.739097	4988.038597	265.983801
214.530747	0.000022	0.000001
215.183525	287.195947	15.490499
215.183525	287.195947	15.490499
219.883464	0.000000	0.000000
219.883464	0.000000	0.000000
221.299698	11887.581684	659.405256
221.299698	11887.581684	659.405256
221.557185	1678.579279	93.219285
222.006652	0.000000	0.000000
222.006652	0.000000	0.000000
226.195751	22108.698911	1253.503925
226.195751	22108.698911	1253.503925
228.675350	0.000000	0.000000
228.675350	0.000000	0.000000
231.193219	0.000004	0.000000
231.799858	625.199771	36.325370
231.799858	625.199771	36.325370
233.182434	320.186498	18.714443
234.165830	0.000000	0.000000
239.572128	1094.427698	65.720587
239.572128	1094.427698	65.720587
240.051174	0.000000	0.000000
240.051174	0.000000	0.000000
241.742761	0.000000	0.000000
241.742761	0.000000	0.000000
244.894036	2415.530065	148.275271

245.521480	2129.935211	131.079252
245.521480	2129.935211	131.079252
247.435693	0.000000	0.000000
247.435693	0.000000	0.000000
248.949312	0.000000	0.000000
248.949312	0.000000	0.000000
254.522504	794.835859	50.708610
254.522504	794.835859	50.708610
254.843168	0.000000	0.000000
254.843168	0.000000	0.000000
256.406191	1003.744404	64.510397
256.406191	1003.744404	64.510397
257.959242	0.000000	0.000000
257.959242	0.000000	0.000000
260.125618	0.000474	0.000031
267.604761	7111.210728	476.996788
267.604761	7111.210728	476.996788
270.312635	3565.214713	241.562829
272.505260	0.000000	0.000000
272.505260	0.000000	0.000000
277.701283	14.894717	1.036784
277.701283	14.894717	1.036784
279.217713	0.000000	0.000000
279.217713	0.000000	0.000000
282.611471	24417.984185	1729.727397
283.000655	12911.639395	915.897553
283.000655	12911.639395	915.897553
288.572020	0.000001	0.000000
294.835759	1991.116950	147.148214
296.275353	0.000000	0.000000
296.275353	0.000000	0.000000
299.654499	24673.834402	1853.256441
299.654499	24673.834402	1853.256441
300.568203	1715.304679	129.229712
309.977604	33358.892137	2591.910530
309.977604	33358.892137	2591.910530

311.216225	0.000000	0.000000
311.216225	0.000000	0.000000
311.769026	930.965609	72.751956
311.769026	930.965609	72.751956
313.562383	0.000032	0.000002
315.324172	0.000000	0.000000
315.324172	0.000000	0.000000
320.178053	0.000000	0.000000
320.178053	0.000000	0.000000
324.505563	24935.577612	2028.241425
330.364684	38267.947861	3168.887775
330.364684	38267.947861	3168.887775
335.549796	841.127319	70.745169
335.549796	841.127319	70.745169
337.960736	0.000000	0.000000
337.960736	0.000000	0.000000
344.206266	17608.427582	1519.208627
344.914019	3954.336138	341.871187
344.914019	3954.336138	341.871187
345.290485	0.000000	0.000000
345.290485	0.000000	0.000000
345.685154	0.000009	0.000001
348.526033	65.332171	5.707427
348.526033	65.332171	5.707427
352.975140	0.000000	0.000000
353.044096	0.000000	0.000000
353.044096	0.000000	0.000000
353.972348	489.780612	43.455925
353.972348	489.780612	43.455925
354.478512	0.000000	0.000000
354.478512	0.000000	0.000000
356.900006	0.000003	0.000000
360.451652	0.000000	0.000000
361.067046	7.639493	0.691402
361.067046	7.639493	0.691402
361.561667	0.000000	0.000000

361.561667	0.000000	0.000000
361.807964	543.143352	49.257307
363.830563	0.000000	0.000000
363.830563	0.000000	0.000000
364.445141	167.867320	15.334739
364.445141	167.867320	15.334739
364.662824	59.828103	5.468583
369.225265	64.793387	5.996532
369.225265	64.793387	5.996532
369.286509	264.159599	24.451635
369.769836	0.000000	0.000000
369.769836	0.000000	0.000000
371.568278	47.869479	4.458363
371.568278	47.869479	4.458363
372.970040	0.000061	0.000006
375.880312	0.000000	0.000000
375.880312	0.000000	0.000000
379.225117	352.929388	33.547718
379.225117	352.929388	33.547718
381.136800	5312.809008	507.555055
381.464356	0.000000	0.000000
381.464356	0.000000	0.000000
383.436549	1826.684831	175.563892
383.436549	1826.684831	175.563892
386.064963	0.000003	0.000000
388.544772	4935.112571	480.635896
388.544772	4935.112571	480.635896
391.764384	1117.329596	109.719627
391.764384	1117.329596	109.719627
395.203032	573.973059	56.857773
399.604531	0.000000	0.000000
405.795187	0.000000	0.000000
405.795187	0.000000	0.000000
407.649388	0.000000	0.000000
407.649388	0.000000	0.000000
423.041454	0.000000	0.000000

423.041454	0.000000	0.000000
429.837576	1040.605124	112.116210
429.837576	1040.605124	112.116210
434.040769	0.000013	0.000001
448.067408	0.000000	0.000000
448.067408	0.000000	0.000000
449.148567	0.000000	0.000000
449.148567	0.000000	0.000000
452.291786	711.589834	80.672684
452.291786	711.589834	80.672684
454.052804	0.000000	0.000000
454.431206	1260.310898	143.556846
454.431206	1260.310898	143.556846
457.678007	1711.522880	196.345442
460.185382	166.373101	19.190841
460.185382	166.373101	19.190841
461.495517	0.000002	0.000000
463.383127	0.000000	0.000000
463.383127	0.000000	0.000000
489.000893	15.868650	1.945036
492.773893	145.300237	17.947009
492.773893	145.300237	17.947009
496.054075	0.000000	0.000000
496.054075	0.000000	0.000000
508.510030	0.000000	0.000000
509.368255	0.000000	0.000000
509.368255	0.000000	0.000000
510.417277	9485.055370	1213.509853
510.417277	9485.055370	1213.509853
515.038078	0.000000	0.000000
525.820502	0.000000	0.000000
525.820502	0.000000	0.000000
529.937567	3.260606	0.433113
531.192305	234.360667	31.204309
531.192305	234.360667	31.204309
537.830142	16.572214	2.234106

542.632622	1897.065172	258.027634
542.632622	1897.065172	258.027634
545.816711	0.000000	0.000000
545.816711	0.000000	0.000000
547.425430	457.693045	62.802561
547.425430	457.693045	62.802561
550.818092	0.000000	0.000000
550.818092	0.000000	0.000000
554.789836	0.000000	0.000000
558.372846	0.000000	0.000000
558.372846	0.000000	0.000000
570.330543	780.009923	111.507692
570.330543	780.009923	111.507692
580.274425	0.000000	0.000000
580.274425	0.000000	0.000000
582.098725	68.970287	10.063215
583.012951	519.336816	75.893640
583.012951	519.336816	75.893640
583.557244	0.000170	0.000025
590.433622	0.000000	0.000000
590.433622	0.000000	0.000000
594.294988	76057.402845	11329.783977
594.294988	76057.402845	11329.783977
629.251315	17414.451884	2746.704958
638.104939	6585.882680	1053.377812
638.104939	6585.882680	1053.377812
646.508745	0.000000	0.000000
646.508745	0.000000	0.000000
647.869017	79457.843803	12903.337517
651.984281	7947.143226	1298.752019
651.984281	7947.143226	1298.752019
654.226553	0.000000	0.000000
654.226553	0.000000	0.000000
665.753421	0.000000	0.000000
671.950698	35709.788096	6014.544645
672.413218	0.000000	0.000000

675.622181	690.625824	116.956613
675.622181	690.625824	116.956613
680.673726	0.000000	0.000000
680.673726	0.000000	0.000000
717.168058	147888.426950	26584.787795
717.168058	147888.426950	26584.787795
740.445836	4996.244784	927.288926
740.445836	4996.244784	927.288926
793.866422	0.000000	0.000000
793.866422	0.000000	0.000000
806.758043	0.000000	0.000000
806.758043	0.000000	0.000000
808.912375	0.000002	0.000000
821.196309	2988.984888	615.245971
830.418941	6820.503470	1419.684207
830.418941	6820.503470	1419.684207
835.420742	4.739621	0.992492
835.420742	4.739621	0.992492
836.448667	0.000000	0.000000
836.448667	0.000000	0.000000
841.712398	0.000000	0.000000
841.712398	0.000000	0.000000
854.664309	0.000000	0.000000
854.664309	0.000000	0.000000
856.527497	0.000000	0.000000
856.527497	0.000000	0.000000
857.256458	8.606940	1.849429
857.256458	8.606940	1.849429
860.473255	84.634564	18.254217
860.473255	84.634564	18.254217
860.879772	16.594307	3.580797
864.108798	0.000000	0.000000
888.777175	0.000000	0.000000
888.777175	0.000000	0.000000
892.129436	16628.459441	3718.415826
892.129436	16628.459441	3718.415826

896.335748	546.813381	122.853610
902.260110	0.000060	0.000014
902.700042	0.000000	0.000000
902.700042	0.000000	0.000000
905.084969	1075.201369	243.925515
905.084969	1075.201369	243.925515
911.496087	40556.990072	9266.134401
916.276074	1.059860	0.243418
916.276074	1.059860	0.243418
926.320310	0.000000	0.000000
926.320310	0.000000	0.000000
929.983191	1421.245702	331.300685
934.199871	14.991356	3.510418
934.199871	14.991356	3.510418
938.024153	0.000000	0.000000
938.024153	0.000000	0.000000
939.058393	0.000000	0.000000
939.067774	469.477472	110.506994
939.067774	469.477472	110.506994
948.989099	0.000000	0.000000
948.989099	0.000000	0.000000
953.722569	0.000000	0.000000
953.722569	0.000000	0.000000
954.543395	1.752891	0.419400
954.543395	1.752891	0.419400
955.533722	0.000005	0.000001
958.437960	2.604367	0.625668
958.437960	2.604367	0.625668
958.866518	0.000001	0.000000
961.843498	0.000000	0.000000
961.843498	0.000000	0.000000
997.544438	0.051645	0.012913
998.968668	1514.717294	379.281379
998.968668	1514.717294	379.281379
1001.036109	0.000000	0.000000
1001.036109	0.000000	0.000000

1066.647368	0.000000	0.000000
1066.647368	0.000000	0.000000
1072.758639	4851.182874	1304.450902
1072.758639	4851.182874	1304.450902
1084.041784	0.000136	0.000037
1120.129192	0.000000	0.000000
1120.129192	0.000000	0.000000
1133.377544	2.032576	0.577430
1133.377544	2.032576	0.577430
1149.685390	17850.853740	5144.179027

Na(H_2O) Preyssler compound

Frequency (degeneracy not counted)	Dipole Strength	Absorption Intensity
cm-1	1e-40 esu2 cm2	km/mole
31.744896	55.890198	0.444721
32.375612	3.150073	0.025563
33.943307	42.488109	0.361493
37.110944	558.446344	5.194713
38.064745	164.210137	1.566755
39.707446	151.367232	1.506544
39.818334	190.774977	1.904068
48.656694	367.204634	4.478461
48.860255	276.670099	3.388411
50.466316	10.627216	0.134431
53.924651	28.472439	0.384849
55.119970	15.923963	0.220008
55.745345	11.681395	0.163223
65.523813	120.179391	1.973819
65.719970	10.978093	0.180843
66.183085	1435.862895	23.819797
66.465959	38.431583	0.640274
66.637109	1284.800805	21.460015
71.771402	273.733527	4.924447
72.473310	743.512711	13.506554

72.881416	728.379530	13.306156
75.333905	47.191715	0.891116
75.877715	492.055884	9.358511
76.004217	243.524588	4.639365
77.268554	1043.069648	20.201991
79.320462	52.531212	1.044433
79.895298	69.855125	1.398935
82.140526	3888.844072	80.067465
82.452634	427.054945	8.826049
82.690761	1518.771299	31.479472
83.687962	7123.093543	149.420337
86.070757	596.199067	12.862488
88.641467	593.314866	13.182574
91.130261	26.269952	0.600067
91.529429	65.318023	1.498552
92.725858	149.265707	3.469277
93.198733	59.888853	1.399053
93.706355	141.892605	3.332782
94.204770	86.659047	2.046279
96.031587	42.299337	1.018183
99.038003	14.410475	0.357732
103.459987	5.926714	0.153697
104.035081	30.402500	0.792806
105.701216	29.409653	0.779198
106.096470	24.263859	0.645266
107.502763	57.102569	1.538698
110.234132	148.733174	4.109623
113.648625	180.061965	5.129373
113.791014	35.336100	1.007870
114.927375	7945.812276	228.896871
117.276063	8396.108676	246.811562
120.663038	15.761018	0.476691
121.171340	12.449884	0.378132
124.043109	92.666051	2.881186
127.430506	1.402425	0.044795
127.646548	11.717858	0.374917

128.803567	64.262353	2.074735
132.326362	79.295860	2.630116
132.461318	139.950531	4.646669
133.269954	13.865305	0.463169
135.814344	1727.211720	58.798912
136.551760	230.427705	7.886968
137.328974	501.365841	17.258180
137.546389	1431.256757	49.345189
137.644780	1112.060836	38.367753
138.294653	1943.814194	67.381117
139.415323	721.025379	25.196437
139.752341	739.069354	25.889422
141.863212	206.730325	7.351095
142.674009	350.918113	12.549566
142.953765	48.983930	1.755203
143.167925	122.478616	4.395255
143.838264	99.741824	3.596084
143.984038	174.265795	6.289333
146.205794	264.707184	9.700819
147.801349	271.834242	10.070723
148.400284	3555.715902	132.263453
149.030794	2631.749673	98.310219
150.110003	200.218821	7.533427
151.080096	607.959305	23.022890
151.095517	726.261797	27.505709
151.314477	550.394987	20.875314
153.684898	625.637945	24.100849
157.221436	208.767239	8.227202
158.108958	827.404287	32.790823
158.292318	13.486232	0.535092
158.890173	9.292344	0.370084
159.671721	299.731194	11.996043
161.852600	18.659177	0.756990
163.837296	4295.687004	176.410110
165.359377	7201.243017	298.479402
167.274143	6229.853797	261.206956

168.105914	1808.299784	76.195881
168.871786	1138.995898	48.212242
169.593054	288.510261	12.264431
169.655536	1108.495675	47.138972
170.766555	742.193949	31.768616
171.147627	207.695825	8.909980
171.465378	4799.339097	206.269942
172.516368	4847.583917	209.620481
173.339644	1183.189289	51.407940
173.888291	777.705026	33.897160
174.846917	13590.721636	595.632746
175.536168	2560.210609	112.647194
176.107912	5659.659770	249.831538
176.511878	1324.377262	58.595427
178.229334	740.945830	33.101198
178.936027	1513.503974	67.882750
179.791023	968.345366	43.639157
180.475102	454.300431	20.551263
181.221933	4423.147639	200.918657
181.566785	3132.586497	142.566519
181.731245	343.956768	15.667927
182.246554	514.003870	23.480308
182.806966	189.531356	8.684641
184.395779	14506.421445	670.485415
186.890281	3396.963765	159.131334
188.340902	51.957371	2.452844
188.950760	25.778414	1.220908
191.619532	213.998339	10.278465
193.111133	4265.859597	206.486632
193.225904	2671.603947	129.394404
194.151156	241.801892	11.767325
194.285131	1535.188142	74.761713
194.706015	526.202934	25.680927
195.434760	14.250101	0.698068
196.643795	1284.165164	63.296428
196.767389	1462.932180	72.153165

200.895320	623.740637	31.408842
201.274752	87.103565	4.394438
201.621101	23.195962	1.172267
203.387384	20.367885	1.038360
203.502628	68.699130	3.504284
203.841390	334.932423	17.113058
204.119543	55.362250	2.832542
204.509353	12.865523	0.659506
205.749234	582.964680	30.064815
206.471355	522.173596	27.024196
206.994521	122.053943	6.332697
207.532392	1931.183484	100.458688
208.164372	3555.085914	185.496009
211.008649	87.173834	4.610675
211.951301	6190.997131	328.908245
212.470662	306.669165	16.332293
212.883032	910.677024	48.594095
213.384278	1396.340623	74.684738
213.577643	36.827073	1.971519
213.865722	234.321034	12.561183
214.273494	86.766370	4.660129
216.582863	4581.153288	248.700687
217.824943	267.505146	14.605547
218.564067	3470.120494	190.108436
219.538563	3820.762796	210.251433
220.140353	7236.428204	399.302460
220.429166	1261.464245	69.698282
220.716874	1963.073468	108.605085
222.115803	16132.609023	898.177428
222.821877	21458.621324	1198.499108
224.445579	11944.155323	671.961773
227.609467	453.565747	25.876685
228.203300	625.668335	35.788555
228.761176	216.864948	12.435113
230.200996	386.024398	22.274093
232.109290	1356.949785	78.946771

233.091163	557.894381	32.595366
235.220025	93.530827	5.514513
236.704236	43.769955	2.596930
238.455127	206.839258	12.362825
239.801095	90.494415	5.439400
240.663662	397.492049	23.978225
241.694328	1060.297302	64.235067
242.389304	717.682442	43.603750
244.186499	70.742944	4.329950
244.708611	446.318760	27.376156
245.649587	2124.896268	130.837381
246.513197	1277.898401	78.961351
249.182714	330.548302	20.645762
250.264121	258.623498	16.223503
250.957600	299.004726	18.808600
252.797977	490.540426	31.083253
255.718822	167.195214	10.716787
257.174187	36.889985	2.378011
258.235504	2105.887760	136.310478
259.622925	1602.779612	104.302548
260.192508	217.777277	14.203174
260.536838	141.594474	9.246844
262.091171	1224.543150	80.446019
263.985387	11037.735291	730.361600
272.786926	11191.104318	765.199302
272.870199	5365.155875	366.958137
273.113931	1325.318929	90.728206
273.421722	2475.061313	169.627807
275.500768	6639.079887	458.467736
277.108107	4183.737503	290.597404
280.760187	882.051027	62.073653
282.628358	3468.055481	245.685679
283.222542	494.244294	35.087106
287.119490	1512.342233	108.840574
288.306976	14.064836	1.016408
290.248811	870.191305	63.308680

293.681434	3093.947614	227.754789
295.699132	15169.054776	1124.311465
296.932638	24472.858150	1821.464450
305.656275	13398.287311	1026.504064
307.783380	5701.085300	439.825873
308.393637	11353.728409	877.651260
309.257354	5747.728231	445.547829
309.319745	17697.869122	1372.166121
309.766672	883.856900	68.626953
310.789801	13914.100541	1083.926829
312.413386	1439.827037	112.750384
312.624094	737.151833	57.764028
314.071522	179.565324	14.136084
314.336776	825.564511	65.046552
316.610570	6243.438524	495.481359
317.486204	670.507910	53.358896
320.146366	240.002873	19.259415
321.113034	361.657038	29.109378
322.799240	2158.994361	174.687601
331.273060	31700.008100	2632.228349
331.492424	29833.650714	2478.894696
334.953761	19903.502334	1671.061496
337.257576	530.594570	44.854145
337.789349	191.491809	16.213405
337.828701	1566.793348	132.674156
338.961168	1789.262935	152.020509
342.519362	3623.961318	311.133483
343.459837	2859.699078	246.192243
344.873848	6192.249577	535.287110
345.298680	462.680024	40.045502
345.394375	2744.043874	237.566052
345.493517	16428.286946	1422.689915
346.221308	10621.843042	921.789469
347.306577	1384.090917	120.491302
350.900077	41.827665	3.678961
351.590377	49.393716	4.352981

352.111943	5.338797	0.471197
353.903788	396.721067	35.192372
354.048698	514.079897	45.621724
354.590220	237.487092	21.107891
354.779448	272.655393	24.246587
354.889469	190.823222	16.974712
359.243056	18.088598	1.628814
359.759694	18.254114	1.646082
360.300925	117.841926	10.642491
361.010507	37.254154	3.371108
361.600221	999.772137	90.616605
361.676536	43.970444	3.986202
363.054643	84.661743	7.704372
363.854328	116.858453	10.657755
363.978033	30.702915	2.801127
365.892616	100.311522	9.199888
366.310302	64.994318	5.967640
368.328659	20.409761	1.884306
369.390495	194.887860	18.044655
370.346235	117.118703	10.872070
370.462586	427.644364	39.710484
371.020607	94.347583	8.774187
372.023701	279.382630	26.052421
372.113379	96.413558	8.992728
372.695367	687.382696	64.214138
380.901745	85.723023	8.184431
381.108005	249.539944	23.837802
382.077386	630.950896	60.426156
382.299213	2511.603016	240.675825
383.706150	3701.322056	355.986645
384.342066	5457.523748	525.764942
385.389106	63.467665	6.130982
385.601698	330.378576	31.932203
387.976847	462.387978	44.966638
389.575126	768.833911	75.076120
390.115204	1049.340478	102.609453

391.791378	591.411838	58.079512
393.510069	130.234059	12.845721
395.702140	132.932066	13.184881
397.912268	448.473610	44.730349
401.125033	26.160875	2.630329
402.970916	4.666113	0.471310
403.223629	3.214379	0.324879
405.959848	2.510761	0.255486
406.356711	1.932528	0.196839
425.019081	84.273825	8.977992
426.800955	30.517444	3.264763
430.967837	1384.784128	149.590842
433.900478	1396.508255	151.883888
436.911682	164.085501	17.969746
442.667163	36.624232	4.063721
444.169448	18.926094	2.107113
446.124719	8.061222	0.901437
446.862942	2.732447	0.306058
448.786784	917.975290	103.264042
449.955764	760.940647	85.822008
452.272772	1102.735350	125.011455
452.974244	1171.783942	133.045173
453.981349	586.695747	66.761951
457.071488	538.330641	61.675304
461.169031	62.448083	7.218672
462.042957	190.959981	22.115807
464.465112	163.192680	18.999048
466.834378	5.181207	0.606278
468.419410	12.464397	1.463471
490.113103	18.651004	2.291272
492.346594	313.992930	38.749748
492.985817	229.776212	28.393410
494.740214	4.499587	0.557992
495.374582	37.755316	4.688025
505.299879	483.797532	61.276071
506.150127	2910.197866	369.215512

507.307712	8152.034844	1036.610401
507.638173	5018.128142	638.519389
509.315624	1980.721512	252.864864
519.151774	15.753241	2.049946
529.280881	12.799194	1.698036
530.033026	186.078104	24.721583
533.979301	108.030534	14.459358
535.011933	179.528509	24.075480
542.346085	6.855810	0.931995
545.604267	45.111198	6.169361
547.960089	43.754561	6.009666
548.562706	34.355511	4.723901
549.834123	159.852947	22.030807
550.319610	32.103914	4.428443
552.517415	1470.094049	203.595962
553.820809	1714.171769	237.958750
556.391875	1374.872637	191.743795
561.410717	59.738419	8.406447
562.464152	7.253631	1.022653
564.467543	14.954033	2.115804
566.775862	1.191985	0.169340
568.454044	12.222580	1.741551
570.626978	92.433531	13.220866
570.995530	167.677694	23.998609
572.657970	67.377121	9.671322
576.440396	806.070921	116.467762
578.948381	10.415815	1.511511
591.237752	2947.961681	436.879897
599.328624	205.270661	30.836847
600.390108	9397.691363	1414.271457
601.032081	5215.556313	785.735478
604.948508	76924.793685	11664.411169
605.037011	71272.208731	10808.868410
631.025582	10936.303863	1729.798853
635.599353	32577.868685	5190.201099
645.604500	6201.283553	1003.520407

645.752365	8222.955491	1330.981487
648.677347	62433.001341	10151.284871
653.066480	187.216297	30.646375
654.369888	404.577744	66.359540
658.652929	7815.482698	1290.299426
659.374023	7856.039287	1298.415078
660.791456	589.207411	97.591207
661.504307	503.019177	83.405615
674.728165	210.880065	35.665017
678.224201	18016.175159	3062.766924
679.381821	2782.666960	473.863462
682.510677	573.233775	98.066187
683.054736	624.365188	106.898659
686.816110	52.341375	9.010807
688.115659	135.323455	23.340631
699.671631	20.441057	3.584889
723.687251	147059.072450	26676.006488
724.502525	145382.533830	26401.597613
743.740735	6324.960683	1179.118543
745.066262	6351.782977	1186.229225
796.562730	7.130091	1.423617
797.029060	5.677771	1.134306
806.281583	9.135860	1.846351
807.904655	9.960704	2.017104
808.548079	17.676550	3.582461
817.870441	3078.207461	631.045202
827.654667	4924.425513	1021.604533
829.004161	5176.349426	1075.618754
832.517903	559.488830	116.751662
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835.934670	9.398512	1.969289
836.150385	5.602326	1.174170
840.179110	6.680565	1.406900
840.279683	1.372301	0.289036
847.329671	23.148961	4.916567
849.271882	4.930465	1.049573

852.148203	0.152285	0.032527
852.762027	0.105055	0.022455
853.426113	17.409895	3.724261
854.033296	20.593690	4.408461
856.921089	38.165512	8.197662
857.241547	55.706542	11.969816
857.583138	56.065102	12.051661
860.763911	3.161559	0.682124
885.333412	169.851765	37.692504
886.046318	175.488216	38.974671
889.955723	15540.622371	3466.688963
890.875504	15808.114817	3530.003770
891.822621	15600.854502	3487.425517
897.326904	960.708776	216.082958
900.536696	5302.871066	1196.990083
901.145362	19171.143971	4330.329570
902.096825	670.803815	151.679451
903.697476	719.381983	162.952376
905.331920	314.369218	71.338819
907.334552	374.779939	85.235763
907.458746	254.468495	57.881394
919.059408	6.399834	1.474315
920.113684	40.351405	9.306325
923.182294	2845.014052	658.339559
927.448373	96.097184	22.339759
928.290264	38.434551	8.943009
932.615073	302.176445	70.638441
932.800540	233.847298	54.676312
933.214967	200.112053	46.809393
933.335764	104.999320	24.564191
933.638024	84.122660	19.686549
944.213319	0.503607	0.119190
944.679884	3.845157	0.910493
950.417114	0.234338	0.055826
951.245379	2.436578	0.580966
951.399946	0.205185	0.048931

951.816274	2.754151	0.657081
953.754580	2.446543	0.584881
955.949298	33.998216	8.146462
956.132712	13.555935	3.248821
957.251156	122.924113	29.494501
960.319754	2.737187	0.658868
960.531036	14.399118	3.466773
996.444563	211.863901	52.916142
997.589178	1484.970220	371.319318
998.085466	1441.920024	360.733915
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1058.391040	132.877034	35.251220
1059.108861	1512.465095	401.517088
1064.165124	3499.677464	933.501699
1066.056428	4682.114726	1251.123883
1074.373395	57.552184	15.498695
1114.874806	345.626886	96.585446
1118.397278	15.254599	4.276367
1132.173942	6.555324	1.860310
1133.843548	1072.147344	304.709277
1147.377039	18304.645226	5264.359519
1580.242449	278.345206	110.251762
3732.654633	123.045502	115.122874
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