

Supporting Information

Vanadium uptake and storage in the fabrication and function of mussel byssus

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Table S1. Tukey post hoc test letter grouping table for the 540 cm⁻¹ resonant peak position.

540 cm ⁻¹ Peak		
Group	Mean	Group letter
Fe-treated	556.05	A
Native	555.51	A B
V-treated	554.29	B

Table S2. Tukey post hoc test letter grouping table for the 590 cm⁻¹ resonant peak position.

590 cm ⁻¹ Peak		
Group	Mean	Group letter
Native	602.01	A
Fe-treated	602.64	A
V-treated	600.69	B

Table S3. Tukey post hoc test letter grouping table for the 640 cm⁻¹ resonant peak position.

640 cm ⁻¹ Peak		
Group	Mean	Group letter
Native	644.98	A
Fe-treated	644.75	A
V-treated	643.43	B

Table S4. Tukey post hoc test letter grouping table for the 1480 cm⁻¹ resonant peak position.

1480 cm ⁻¹ Peak		
Group	Mean	Group letter
Native	1479.91	A
Fe-treated	1478.87	B
V-treated	1477.48	C

Figure S1. Boxplots showing the distribution of Raman shift peak positions for four of the metal-DOPA resonant peaks after metal-loading experiments.

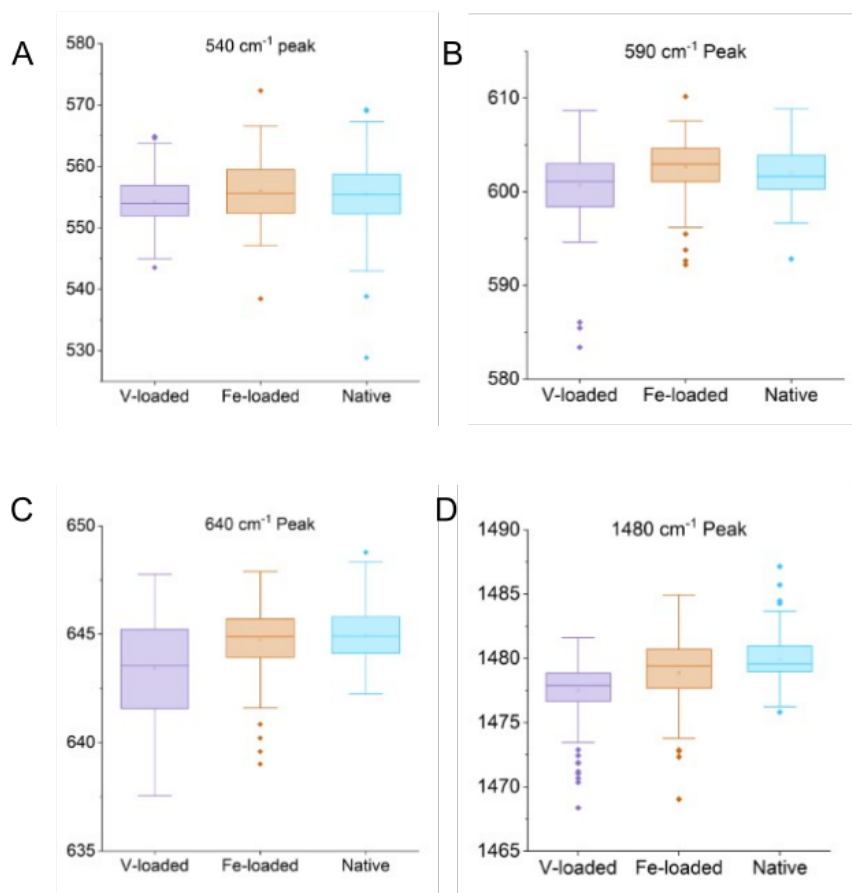


Table S5. $[\text{V}(\text{cat})_3]^{2-}$ vibrational modes^a, cc-PVTZ, B3LYP

Mode number	Frequency (cm^{-1})	Infrared ^b activity	Raman ^c activity	Depolar-P ^d	Depolar-U ^d
1	26.35	0.0392	21.811	0.75	0.8571
2	26.44	0.0394	21.7853	0.75	0.8571
3	54.53	0.154	0.0017	0.7401	0.8507
4	67.36	0.0043	6.9063	0.75	0.8571
5	67.52	0.0045	6.9721	0.75	0.8571
6	69.61	0	11.2627	0.7347	0.8471
7	150.8	0.3486	0	0.7037	0.8261
8	175.63	0.0122	0.9168	0.75	0.8571
9	175.64	0.0125	0.9071	0.75	0.8571
10	216.66	0.0001	61.66	0.1455	0.2541
11	220.6	0.1265	1.465	0.73	0.844
12	220.64	0.1424	0.5069	0.7451	0.8539

14	229.07	0.1464	0.4962	0.7492	0.8566
15	233.63	0	73.3909	0.0786	0.1457
16	310.78	11.9267	0	0.2043	0.3392
17	326.27	11.1682	6.6378	0.75	0.8571
18	326.29	11.1703	6.619	0.75	0.8571
19	363.24	22.0614	0	0.643	0.7827
20	420.49	96.1125	84.3857	0.75	0.8571
21	420.53	96.1715	84.3142	0.75	0.8571
22	456.41	0.1203	0.001	0.7308	0.8444
23	460.08	9.4864	13.6828	0.75	0.8571
24	460.14	9.5356	13.7011	0.75	0.8571
25	509.62	190.8363	12.5309	0.75	0.8571
26	509.68	190.722	12.5737	0.75	0.8571
27	539.86	23.0429	0.8406	0.7499	0.8571
28	539.88	23.0778	0.843	0.7488	0.8564
29	546.27	0.0006	103.5251	0.1278	0.2266
30	556.21	8.5082	0	0.34	0.5075
31	580.07	0.0552	0.1771	0.7484	0.8561
32	580.1	0.0552	0.1831	0.7113	0.8313
33	580.46	0.0002	2.5148	0.1167	0.209
34	611.95	0.0098	14.419	0.75	0.8571
35	611.97	0.0111	14.3985	0.75	0.8571
36	623.62	24.6709	0.0007	0.232	0.3767
37	631.81	208.8342	58.3652	0.7498	0.857
38	631.84	208.9867	58.3458	0.7499	0.8571
39	634.15	0.0074	424.8396	0.0824	0.1523
40	709.4	34.567	0.0196	0.75	0.8571
41	709.66	71.3656	1.5695	0.75	0.8571
42	709.71	71.1978	1.5631	0.75	0.8571
43	743.3	0.0416	0.3212	0.7357	0.8477
44	743.32	0.0429	0.3158	0.7489	0.8564
45	743.6	0.0001	3.6715	0.2903	0.4499
46	817.63	51.1175	1.9875	0.75	0.8571
47	817.64	51.0664	1.9849	0.75	0.8571
48	820.55	0.0002	23.4099	0.1343	0.2368
49	832.39	0.2144	0.1646	0.7458	0.8544
50	832.41	0.2128	0.1658	0.7448	0.8538
51	832.76	0.0004	1.4751	0.2162	0.3555
52	867.77	5.887	0.0012	0.7482	0.8559
53	868.03	17.9329	0.3656	0.75	0.8571
54	868.05	17.9437	0.3669	0.75	0.8571
55	877.51	0.0064	0.0249	0.7354	0.8476
56	877.54	0.0048	0.0362	0.7227	0.8391

57	877.58	0.0021	0.0715	0.7099	0.8303
58	886.34	10.3309	17.4045	0.75	0.8571
59	886.34	10.3377	17.4011	0.75	0.8571
60	891.76	31.2344	0	0.1872	0.3154
61	1029.93	44.9505	3.5577	0.7404	0.8508
62	1029.95	44.9671	3.5427	0.7467	0.855
63	1030.53	0.0271	59.2415	0.0001	0.0002
64	1106.14	3.2912	0.2609	0.75	0.8571
65	1106.16	3.2448	0.2611	0.75	0.8571
66	1106.35	25.5676	0.0007	0.7495	0.8568
67	1154.99	1.1696	27.9111	0.7481	0.8559
68	1155	1.1651	27.8739	0.75	0.8571
69	1155.25	0.0006	83.5264	0.0203	0.0398
70	1248.36	0.1424	5.2129	0.75	0.8571
71	1248.38	0.1415	5.2086	0.75	0.8571
72	1249.14	8.0317	0.0018	0.7491	0.8566
73	1294.27	804.572	237.3995	0.75	0.8571
74	1294.28	805.9971	237.4786	0.75	0.8571
75	1301.13	62.3139	2.9465	0.749	0.8565
76	1301.15	64.8247	3.1824	0.7498	0.857
77	1308.96	5.8541	0.0188	0.1232	0.2194
78	1314.41	0.0001	989.2231	0.1022	0.1854
79	1374.28	31.254	305.3321	0.75	0.8571
80	1374.31	31.2571	305.1775	0.7496	0.8569
81	1375.64	0.0039	915.0554	0.1172	0.2098
82	1471.29	1.1855	5.8077	0.75	0.8571
83	1471.34	1.202	5.8241	0.75	0.8571
84	1473.5	1.5522	0.0021	0.4443	0.6153
85	1502.51	383.3384	835.6203	0.75	0.8571
86	1502.55	383.1508	835.8682	0.75	0.8571
87	1511.15	0.0027	2751.5026	0.118	0.2111
88	1580.35	16.4229	101.8891	0.75	0.8571
89	1580.36	16.4056	101.961	0.75	0.8571
90	1586.52	21.835	0.0006	0.5502	0.7098
91	1594.08	14.0545	12.2631	0.7499	0.8571
92	1594.09	14.0164	12.2791	0.7499	0.8571
93	1594.57	0.0043	17.2402	0.3317	0.4982
94	3106.29	3.2572	124.3313	0.75	0.8571
95	3106.31	2.9417	126.8255	0.75	0.8571
96	3106.34	16.7181	19.7795	0.75	0.8571
97	3126.55	142.0859	261.4359	0.7481	0.8559
98	3126.57	141.8124	261.8342	0.7454	0.8541
99	3126.76	0.7591	534.3331	0.2944	0.4549

100	3146.6	28.4256	131.5636	0.7499	0.8571
101	3146.64	32.138	129.9132	0.75	0.8571
102	3146.86	226.1507	4.1569	0.75	0.8571
103	3152.88	108.0629	113.8415	0.7483	0.856
104	3152.91	107.4153	115.0805	0.7428	0.8524
105	3153.69	0.0963	929.4497	0.025	0.0487

- a. C_1 point symmetry
- b. IR Activity in KM/mol
- c. Raman activity $\text{\AA}^4/\text{AMU}$
- d. Depolarization ratios

Table S6. $[\text{Fe}(\text{cat})_3]^{3-}$ vibrational modes^a, cc-PVTZ, B3LYP

Mode number	Frequency (cm ⁻¹)	Infrared ^b Activity	Raman ^c Activity	Depolar-P ^d	Depolar-U ^d
1	26.76	0.0065	19.2172	0.75	0.8571
2	26.95	0.0068	19.1258	0.75	0.8571
3	45.78	0.0037	0.001	0.7482	0.856
4	58.13	0.0285	7.0287	0.75	0.8571
5	58.91	0.028	7.1502	0.75	0.8571
6	65.66	0.0001	11.7491	0.7457	0.8543
7	131.03	0.0324	0.0001	0.2167	0.3562
8	156.8	0.2561	2.974	0.75	0.8571
9	156.85	0.2621	2.9805	0.75	0.8571
10	168.95	0.5142	0.221	0.7488	0.8564
11	169.05	0.5019	0.2179	0.7495	0.8568
12	179.15	0	108.3624	0.135	0.2379
13	199.4	0.0759	5.552	0.7489	0.8564
14	199.65	0.0776	5.5219	0.7499	0.857
15	207.85	0.0001	31.886	0.0455	0.087
16	242.12	36.3547	0.0002	0.199	0.3319
17	293.78	153.3847	20.0123	0.75	0.8571
18	293.85	152.9398	19.9555	0.75	0.8571
19	308.91	0.3282	0.0001	0.709	0.8297
20	331.04	91.6672	23.7354	0.75	0.8571
21	331.14	91.9608	23.8188	0.75	0.8571
22	457.9	0.1512	0.0019	0.7389	0.8498
23	459.4	0.4478	1.081	0.75	0.8571
24	459.49	0.4601	1.0881	0.7499	0.8571
25	477.03	103.9167	28.7528	0.75	0.8571
26	477.05	103.9692	28.7711	0.75	0.8571
27	498	0.0001	163.6887	0.1173	0.21
28	505.28	2.6065	0.527	0.746	0.8545
29	505.36	2.607	0.5306	0.7493	0.8567
30	515.22	2.4979	0.0001	0.5536	0.7126
31	544.73	0.043	0.6495	0.7403	0.8508
32	544.75	0.0429	0.6616	0.7101	0.8305
33	544.89	0.0006	2.2826	0.0889	0.1632
34	597.06	4.5632	8.6282	0.7499	0.8571
35	597.09	4.2023	8.8685	0.7498	0.857
36	598.2	5.4461	0.0147	0.7328	0.8458
37	599.56	62.2371	23.457	0.7499	0.8571
38	599.59	61.8773	23.6917	0.75	0.8571

39	604.17	0.0002	193.4576	0.0692	0.1294
40	660.47	30.7815	0.3296	0.75	0.8571
41	660.81	54.9749	4.1026	0.75	0.8571
42	660.91	57.0017	4.4121	0.75	0.8571
43	698.13	0.1542	1.0296	0.5989	0.7492
44	698.19	0.1327	1.6275	0.5229	0.6867
45	698.26	0.0375	5.4804	0.4405	0.6116
46	784.03	2.4482	1.8616	0.7492	0.8566
47	784.04	2.4383	1.86	0.7498	0.857
48	785.35	0.0001	38.5357	0.0185	0.0364
49	811.17	0.1425	1.7332	0.672	0.8038
50	811.3	0.144	1.6856	0.7388	0.8498
51	811.44	0.0164	2.2631	0.2196	0.3602
52	818.51	15.8124	0.0293	0.75	0.8571
53	819.2	33.6403	1.7611	0.75	0.8571
54	819.31	33.9228	1.7791	0.75	0.8571
55	822.93	0.0498	0.0907	0.1505	0.2616
56	822.95	0.0372	0.1731	0.1538	0.2667
57	823	0.0299	0.2416	0.1532	0.2657
58	885.87	13.9998	20.194	0.75	0.8571
59	885.89	13.9799	20.2033	0.75	0.8571
60	889.59	55.8435	0.0002	0.7336	0.8463
61	1026.68	48.9314	3.0963	0.7485	0.8562
62	1026.69	48.9686	3.0982	0.7483	0.8561
63	1027.25	0.0084	46.3319	0.0045	0.0089
64	1089.83	7.1304	0.8461	0.75	0.8571
65	1089.9	5.5741	0.9016	0.75	0.8571
66	1089.99	30.4707	0.0826	0.7498	0.857
67	1139.51	3.1186	17.1207	0.3614	0.5309
68	1139.58	3.516	12.3415	0.7195	0.8369
69	1139.63	0.4583	47.4193	0.0144	0.0283
70	1235.38	0.8894	0.2131	0.75	0.8571
71	1235.45	0.6097	0.234	0.75	0.8571
72	1235.5	2.9684	0.0432	0.75	0.8571
73	1302.38	986.425	0.2635	0.7471	0.8552
74	1302.42	986.3534	0.2609	0.7498	0.857
75	1321.04	0.0011	156.7014	0.1104	0.1988
76	1326.01	6.2591	0.2483	0.7482	0.856
77	1326.07	6.3708	0.254	0.7469	0.8551
78	1330.98	19.4021	0.0002	0.1074	0.194
79	1357.54	102.1748	281.6387	0.7497	0.8569

80	1357.58	102.3315	281.5852	0.7499	0.8571
81	1359.9	0.0148	939.3981	0.1166	0.2089
82	1456.26	2.2349	9.6568	0.75	0.8571
83	1456.33	2.2311	9.6603	0.75	0.8571
84	1458.07	1.462	0.0069	0.7156	0.8343
85	1515.37	870.313	810.3455	0.75	0.8571
86	1515.38	871.0246	810.3938	0.75	0.8571
87	1527.97	0.0014	3728.133	0.1054	0.1906
88	1549.34	20.9762	161.6298	0.75	0.8571
89	1549.35	21.2236	161.1464	0.75	0.8571
90	1554.8	75.1937	0.0063	0.2007	0.3343
91	1568.82	28.2356	4.1023	0.7499	0.8571
92	1568.84	28.142	4.1206	0.7495	0.8568
93	1569.32	0.0086	3.728	0.1821	0.3081
94	3054.99	5.9285	173.6292	0.75	0.8571
95	3055.01	13.577	129.8415	0.75	0.8571
96	3055.06	25.3645	63.0427	0.75	0.8571
97	3079.91	280.4427	291.1623	0.7474	0.8555
98	3079.96	279.7737	292.6659	0.7428	0.8525
99	3080.31	2.029	637.7959	0.285	0.4436
100	3106.69	68.9638	112.3333	0.75	0.8571
101	3106.8	60.1792	114.9857	0.75	0.8571
102	3107.12	428.1522	3.4345	0.7493	0.8567
103	3114.86	150.9566	140.9911	0.7311	0.8446
104	3114.94	150.6563	139.4222	0.7493	0.8567
105	3115.99	0.3355	987.0647	0.0302	0.0586

- a. C_1 point symmetry
- b. IR Activity in KM/mol
- c. Raman activity $\text{\AA}^4/\text{AMU}$
- d. Depolarization ratios