# Supporting Information

Application of group V polyoxometalate as efficient base catalyst: a case study of decaniobate cluster

Shun Hayashi[†], Seiji Yamazoe[*,†,‡], Kiichirou Koyasu[†,‡], and Tatsuya Tsukuda[*,†,‡]

[†]*Department of Chemistry, School of Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-Ku, Tokyo 113-0033, Japan*

[‡]*Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Katsura, Kyoto 615-8520, Japan*

Table S1. Cartesian coordinates of the calculated $[Nb_{10}O_{28}]^{6-}$ structure.
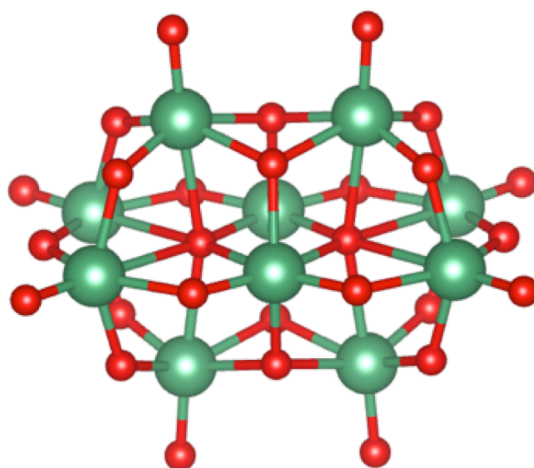
Green and red spheres represent Nb and O, respectively.

Atom	X (Å)	Y (Å)	Z (Å)
Nb	0.002517	0.001696	−1.723302
Nb	−0.002419	−0.001701	1.723192
Nb	1.702047	−2.478433	0.000966
Nb	−3.38787	0.001388	−1.745362
Nb	3.387111	−0.000023	−1.745166
Nb	−3.386708	−0.001839	1.745193
Nb	−1.702172	2.478326	0.001572
Nb	1.702036	2.477601	0.000646
Nb	−1.702202	−2.47749	−0.003307

Nb	3.387656	0.000487	1.745529
O	−1.380214	−0.001201	0.003636
O	1.37986	0.001245	−0.003432
O	−0.002444	2.004534	−1.267005
O	0.000902	2.007537	1.261955
O	0.003078	−2.004472	1.266991
O	−0.001423	−2.007595	−1.26198
O	−2.912812	1.91782	−1.419056
O	−2.91191	1.917799	1.420199
O	2.909961	1.917393	−1.422175
O	2.914256	1.919925	1.418029
O	−2.915031	−1.919443	−1.418811
O	−2.909321	−1.918145	1.421607
O	2.911001	−1.918135	−1.419521
O	2.913502	−1.917263	1.419611
O	−4.322017	−0.000608	0.000677
O	4.321967	0.000589	−0.000659
O	−1.545287	−0.002932	−2.790264
O	1.54301	−0.002382	−2.797344
O	−1.542981	0.002392	2.797399
O	1.545303	0.002884	2.790417
O	−1.833602	4.260166	0.000883
O	1.831806	4.259626	−0.001738
O	−1.831661	−4.259531	−0.001369
O	1.83376	−4.260256	0.001823
O	−4.67686	0.002202	−3.003053
O	4.676363	−0.000453	−3.0027
O	−4.675802	−0.002571	3.002826
O	4.676616	0.000822	3.003252

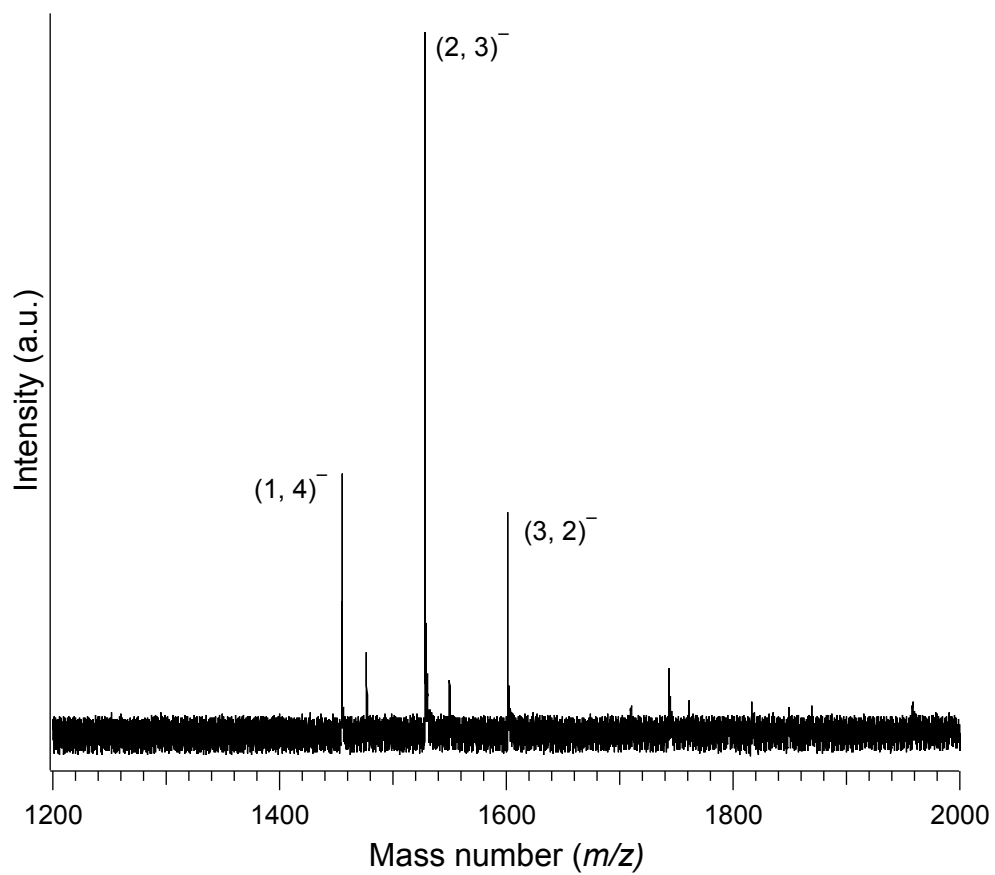**Figure S1.** ESI-MS of $(TMA)_6[Nb_{10}O_{28}] \cdot 6H_2O$ after the reaction (entry 2-1 of Table 1). Peaks for $(TMA)_xH_y[Nb_{10}O_{28}]^-$ are noted as $(x, y)^-$.
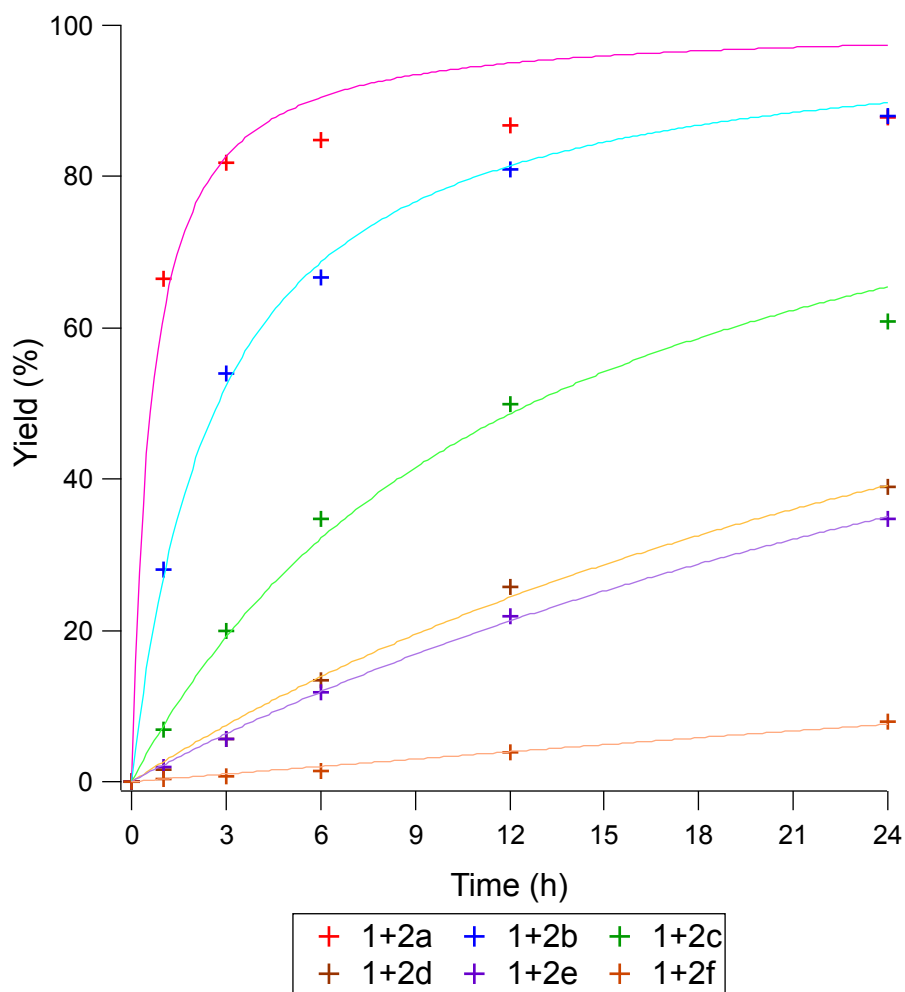
Figure S2. Time course of Knoevenagel condensation reactions at 343 K. Fitted curves were obtained by assuming that the coulpling of nitriles with aldehyde was the rate-determining step and that the reactions followed irreversible second-order kinetics.