

Supplementary information for:

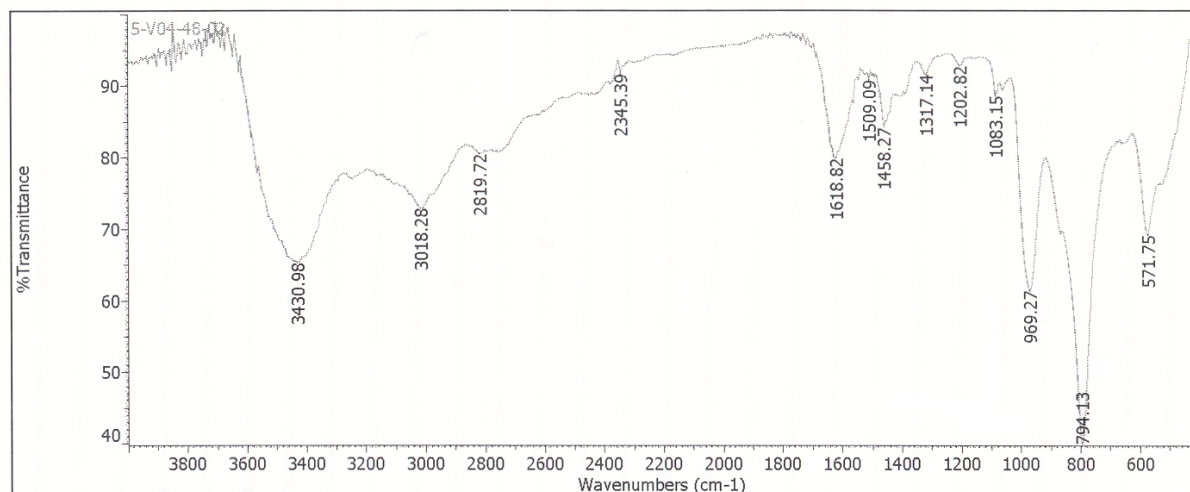
**Re-determination of the Structure of an Anionic
Oxo-vanadium Arsenate Framework**

by

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Infrared spectrum
Elemental analysis

Supplementary Material (ESI) for Dalton Transactions
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 IR spectrum of complex 1 with $[(As_6V_{12}V_3O_{51})_n]_{\infty}$ framework formula



Peak finding results for: 5-V04-48-02

Frequency: 406.75 - 3993.25, threshold: 99.216-95.000, sensitivity: 59.00

Peak finding result table:

Peak#	1	2	3	4	5	6	7	8
Position	3904.99	3872.76	3855.45	3840.69	3822.89	3803.30	3770.92	3752.72
Height	92.731	92.855	91.902	93.204	93.676	94.377	94.964	94.224
Peak#	9	10	11	12	13	14	15	16
Position	3677.83	3650.83	3630.51	3430.98	3018.28	2819.72	2345.39	1618.82
Height	94.917	94.038	91.787	65.076	72.682	80.379	91.490	79.683
Peak#	17	18	19	20	21	22	23	24
Position	1509.09	1458.27	1317.14	1202.82	1083.15	969.27	794.13	571.75
Height	90.636	83.999	91.465	92.734	88.407	61.208	39.703	68.959

The IR spectrum of complex 1 exhibits the following prominent band, in cm^{-1} : For the extra-framework species, O-H and N-H stretching vibrations from the water and piperazinium ions; N-H bending vibrations around 1620, and C-N and C-H vibrations of the piperazinium ion in the region 1000 to 1500. For the framework, terminal V=O vibrations around 960, As-O vibrations around 800.

The spectrum was recorded on a Thermo Scientific Nicolet IR100 FT-IR instrument. Complex 1 was dispersed in a KBr pellet. 16 scans were recorded on the complex, and the background spectrum subtracted.

August 22, 2008**Revised Report 9/16/08****Client:** VIRGINIA TECH
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Blacksburg, VA 24061**Attn:** Vicki Soghomonian**Project:** P9018684**Date Received:** August 18, 2008**Certificate of Analysis**

Sample ID:	Lab #:		Carbon %	Hydrogen %	Nitrogen %	Arsenic %	Vanadium %
V04-29-14	13085		7.00	3.58	4.29	16.5	26.5
duplicate			6.93	3.27	4.27	16.0	25.1

4-6 Day Rush**Notes:****CHN analyzed with WO_3 catalyst. Replicate CHN verifies reported values.****Revised Report 9/16/08: Reported duplicate values that were analyzed during the original analyses.**

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