Electronic Supplementary Material (ESI) for Catalysis Science & Technology.


# Supporting information

## Structural characterization of vanadium environments in MCM-41 molecular sieve catalysts by solid state $^{51}V$ NMR

Marcos de Oliveira, Jr.,[1] Dominik Seeburg,[2] Jana Weiß,[2] Sebastian Wohlrab,[2] Gerd Buntkowsky,[1*] Ursula Bentrup,[2*] Torsten Gutmann [1, 3*]

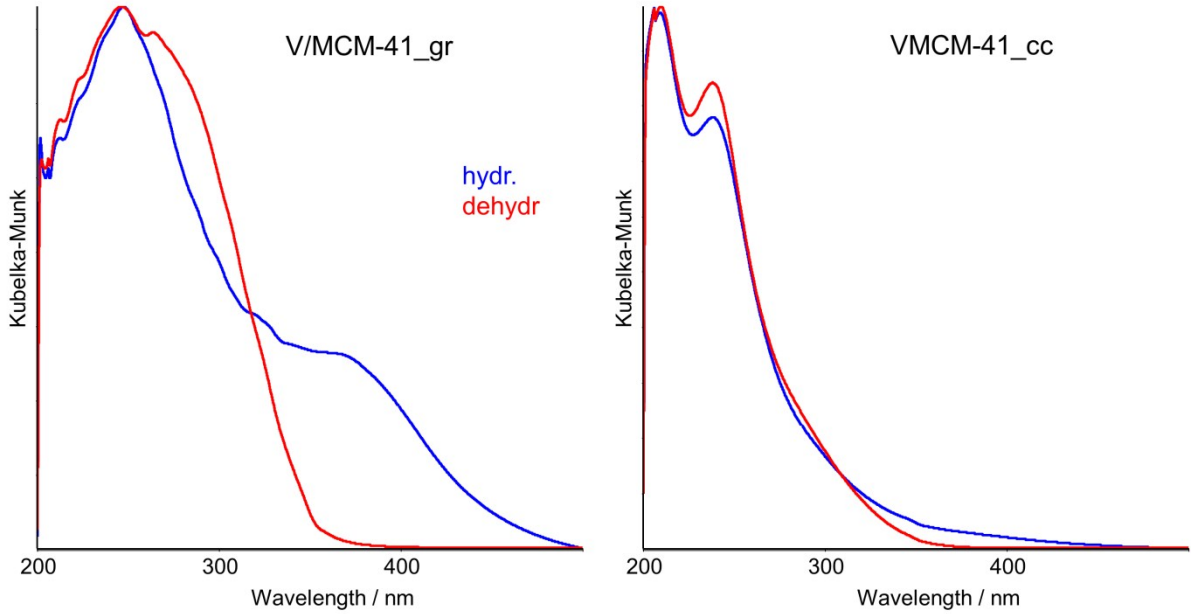
[1] *Institut für Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany*

[2] *Leibniz-Institut für Katalyse e. V. an der Universität Rostock (LIKAT), Albert-Einstein-Str. 29a, 18059 Rostock, Germany*

[3] *Institute of Chemistry and Center for Interdisciplinary Nanostructure Science and Technology, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany.*

*Corresponding authors:* *ursula.bentrup@catalysis.de*
*gerd.buntkowsky@chemie.tu-darmstadt.de*
*gutmann@chemie.tu-darmstadt.de*

(A)




(B)

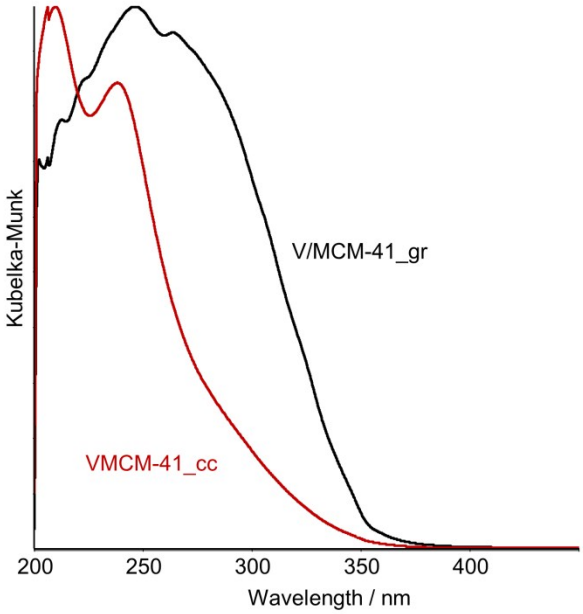



**Figure S1.** Normalized UV-vis DR spectra of VMCM-41_cc and V/MCM-41_gr measured at room temperature before (hydr.) and after 30 min heating in synthetic air at 350°C (A) and direct comparison of the spectra of the dehydrated samples (B).

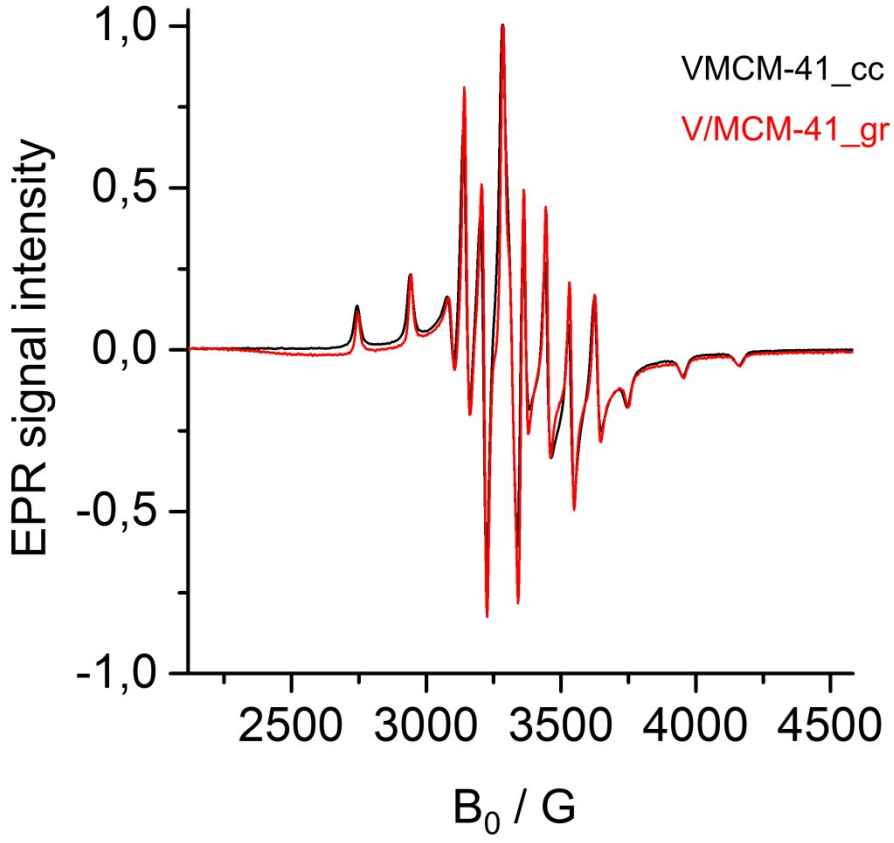



**Figure S2.** Normalized X-band EPR spectra of the dehydrated samples V/MCM-41_gr and VMCM-41_cc measured at -173°C. For both samples signals with well-defined hyperfine structure are observed, with $g_{\perp} = 1.977$ and $g_{||} = 1.931$ and hyperfine coupling constant $A_{\perp} = 76$ and $A_{||} = 203$G. These parameters can be attributed to well isolated $V^{4+}$ units.[1]

**References**

1 C. B. Rodella, R. W. A. Franco, C. J. Magon, J. P. Donoso, L. A. O. Nunes, M. J. Saeki, M. A. Aegerter, V. Sargentelli and A. O. Florentino, *J. Sol-Gel Sci. Technol.*, 2002, **25**, 83–88.