

Supporting information for

Retrosynthetic approach to design of molybdenum-magnesium oxoalkoxides

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Crystal structure details.

Notes on **2**: Solvate molecules located between the organometallic parts are disordered. Although we were able to find separate partially occupied DMFA moieties they overlapped heavily with randomly distributed residual peaks. Therefore the whole part of the solvent was removed using the SQUEEZE procedure implemented in PLATON package [1]. We were unable to find hydrogen atoms of the methanol moieties coordinating the Mg atom. However, the Mg-O distances in these fragments are closer to the alcohol values than to deprotonated ones (typical for Me-O-Mg: 2.0 Å, for Me-OH-Mg: 2.1 Å). Moreover, the disposition of the corresponding atoms O(7S) and O(8S) are typical for intermolecular H-bond formation. For O(9S) there is no hydrogen acceptor, but the distance Mg-O indicates that the moiety should be protonated. Most probably the corresponding H-bond is formed with the disordered solvent molecule eliminated by SQUEEZE procedure. Based on the above reasoning, we have added three H atoms to the MeOH moieties coordinating the cation. An additional note should be made of the disordered O7S-C102 / methanol moiety. We are not sure about the coordination on this site, since fully occupied MeOH does not fit to the model (C-O distance is too long for the methanol). We suggest that this coordination position is partially occupied with water molecules, but since the disordered solvent was removed by SQUEEZE, the refined relative ratios are in somewhat arbitrary. In any case, the suggested model lead to lower R-factor values. Anisotropic refinement of the disordered parts lead to N.P.D. thermal ellipsoids, therefore these moieties were refined in isotropic approximation. One of the coordinated DMFA molecules was refined in rigid-body approximation with relative occupancy of the two components of ca. 1:1.

Notes on **4b**: one of the two methanol molecules is heavily disordered and its contribution to the diffraction was eliminated with SQUEEZE procedure. The hydrogen atoms of the second solvate methanol molecule were not located due to apparent disorder of both C and O atoms.

Notes on **5a**: The crystal was non-merohedrally twinned. The relative orientation of the components was found with CELL_NOW program [2] program and the structure was refined as a twin (SHELX HKLF 5 instruction) with a relative batch scale factor refined to be of 0.385.

IR-spectra of the complexes.

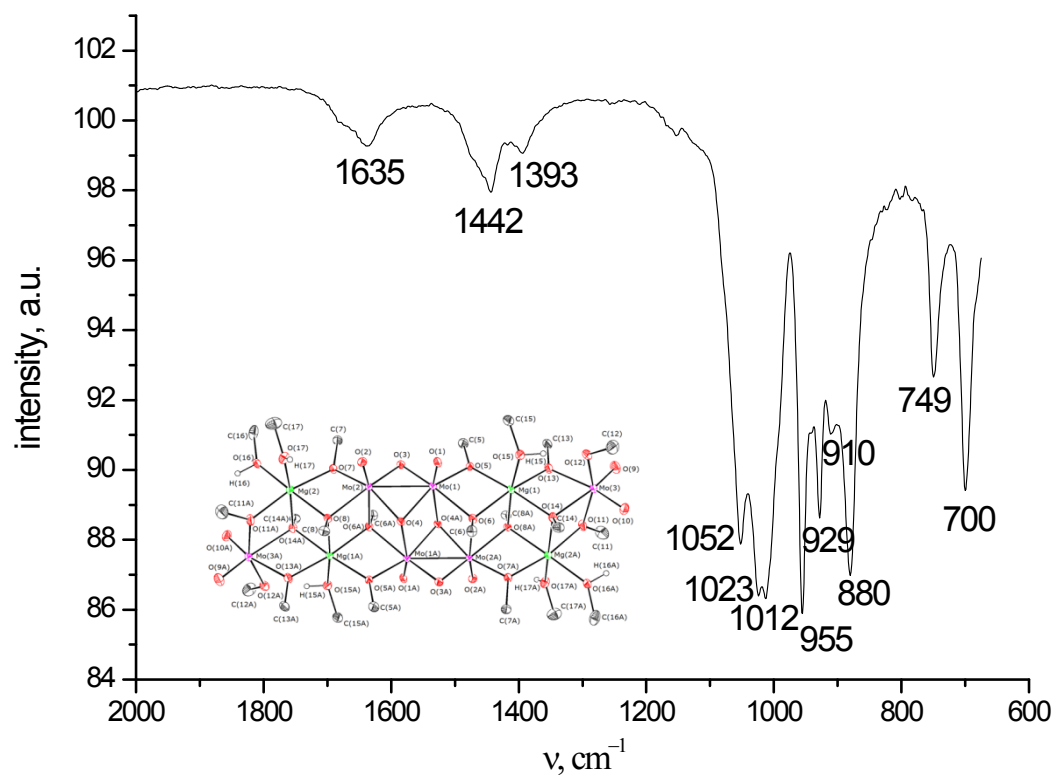


Fig. S1 IR-spectrum of 3.

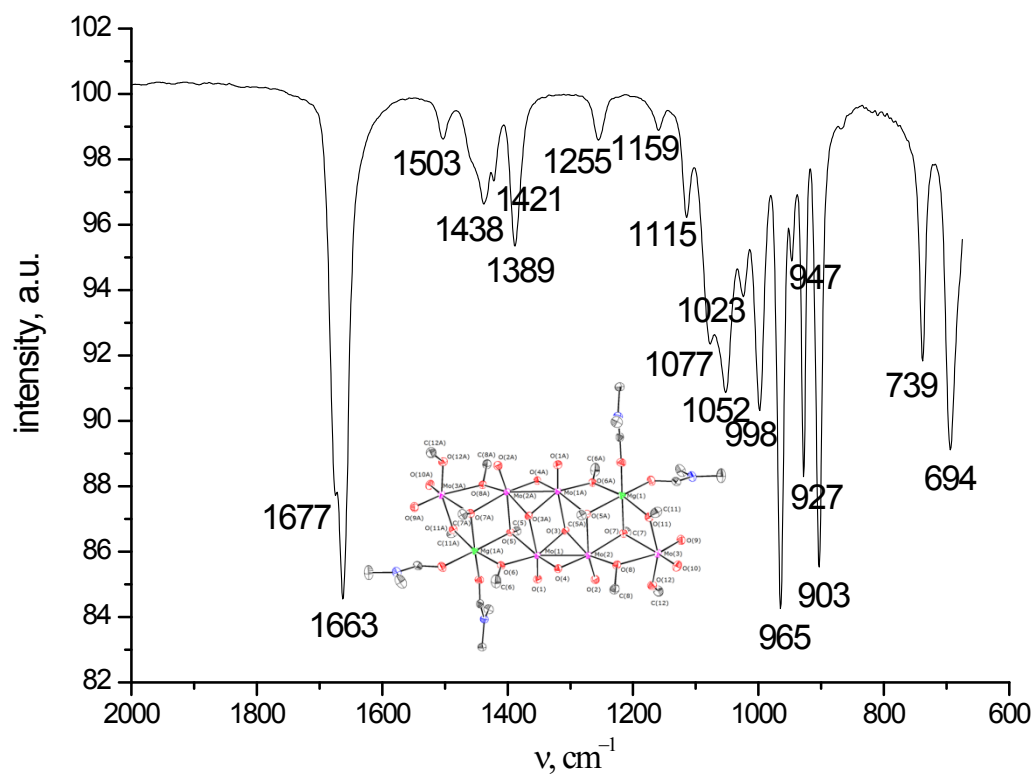


Fig. S2 IR-spectrum of **4a**.

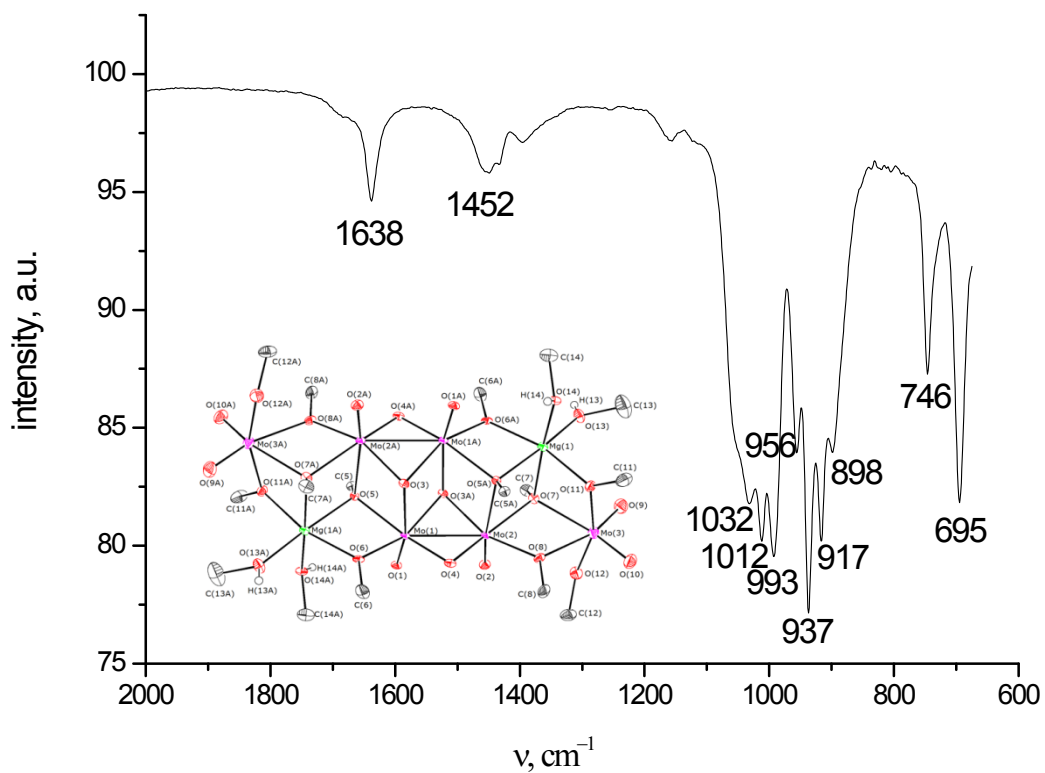


Fig. S3 IR-spectrum of **4b**.

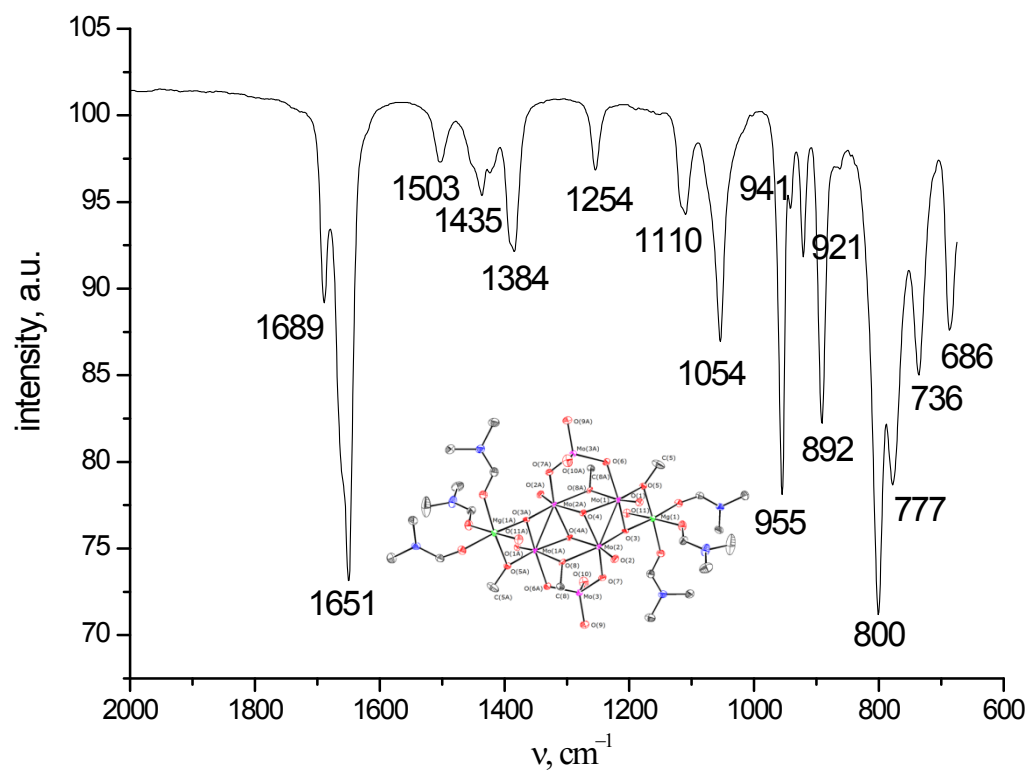


Fig. S4 IR-spectrum of 5a.

References:

- [1] A.L. Spek, *Acta Cryst.*, 2009, **D65**, 148-155.
- [2] G.M. Sheldrick, CELL_NOW v2008/2 - Program for unit cell determination, 2008.