**MAS NMR experiment and GIPAW calculation: N=C-N 13C and OH···O 1H chemical shifts**

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In the following, the names of all raw data files from the solid-state NMR measurements and different calculations are presented:

1. **Raw files for the PXRD experiments**

**Figure S1:** PXRD data recorded on a Panalytical X’Pert Pro MPD equipped with a curved Ge Johansson monochromator, λ = 1.541 Å:

1. **EC029\_5-50-6hr25.xy** (recorded on 24/02/2018)
2. **EC046\_5-50-5hr25\_1.xy** (recorded on 23/08/2018)
3. **EC087\_4-50-1hr38\_1.xy** (recorded on 15/03/2019)
4. **EC037\_5-50-16hr\_1.xy** (recorded on 21/05/2018)
5. **Raw files from NMR experiments**

**Figure 3:** 1H (600 MHz) one-pulse MAS (60 kHz):

**(top left)**26L:F: **Figure 3 [1]** (recorded 30/03/2018)

**(top right)** 25L:FFA: **Figure 3 [2]** (recorded 01/10/2018)

**(bottom left)**26AMP:F-H2: **Figure 3 [3]** (recorded 01/10/2018)

**(bottom right)** 25AMP:FFA: **Figure 3 [4]** (recorded 01/10/2018)

**Figure 4:** 14N-1H HMQC MAS (60 kHz) NMR spectra:

**(top left)**26L:F: **Figure 4 [1]** (recorded 28/05/2017)

**(top right)** 25L:FFA: **Figure 4 [2]** (recorded 01/10/2018)

**(bottom left)**26AMP:F-H2: **Figure 4 [3]** (recorded 26/03/2019)

**(bottom right)** 25AMP:FFA: **Figure 4 [4]** (recorded 01/08/2018)

**Figure 5:** 1H-13C CP-MAS (12.5 kHz) spectra:

**(top left)**26L:F: **Figure 5 [1]** (recorded 25/08/2017)

**(top right)** 25L:FFA: **Figure 5 [2]** (recorded 24/05/2019)

**(bottom left)**26AMP:F-H2: **Figure 5 [3]** (recorded 23/01/2019)

**(bottom right)** 25AMP:FFA: **Figure 5 [4]** (recorded 07/06/2018)

**Figure S3:** 1H-13C CP-MAS (12.5 kHz) spectra:

**(left)**26AMP:F-H2: **Figure S3 [1]** (recorded 06/04/2019)

**(right)** 25AMP:FFA: **Figure 5 [2]** (recorded 18/06/2018)

1. **For the calculations, the initial CIF file, the CIF file after geometry optimisation and the magres-files for the full crystal structure and isolated molecules**

MIBYEB.cif (as determined by single-crystal X-ray diffraction)

MIBYEB\_opt.cif

MIBYEB\_NMR.magres

DUTNUC.cif (as determined by single-crystal X-ray diffraction)

DUTNUC\_opt.cif

DUTNUC\_NMR.magres

COGCIN.cif (as determined by single-crystal X-ray diffraction)

COGCIN\_opt.cif

COGCIN\_NMR.magres

RESGEC.cif (as determined by single-crystal X-ray diffraction)

RESGEC\_opt.cif

RESGEC\_NMR.magres

FUMAAC.cif (as determined by single-crystal X-ray diffraction)

FUMAAC\_opt.cif

FUMAAC\_NMR.magres