

Magn. Reson. Discuss., author comment AC1
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Reply on RC1

César Leroy et al.

Author comment on "A novel multinuclear solid-state NMR approach for the characterization of kidney stones" by César Leroy et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-38-AC1>, 2021

We want to thank the anonymous reviewer for his/her helpful comments. *We answer all questions/comments below.*

- Page 7, line 168. I do not understand the sentence 'from one synthetic sample (Shepelenko 2019)'. Does this mean that the COM synthesis is not perfectly reproducible?

The synthesis is perfectly reproducible in the sense that COM is always obtained by using the described synthetic protocol. No COD or COT were obtained. However, the detailed structure of the obtained COM includes a degree of subtlety. It can evolve from an ordered structure (space group $P2_1/c$) mainly described in the literature and a so-called disordered phase exhibiting a statistical $I2/m$ space group (Shepelenko, 2019) (with a priori different NMR characteristics - NB: the powder XRD patterns are almost identical with tiny differences hardly discernable). The relative energies of both phases are comparable meaning that the final COM structure depends strongly on the experimental conditions. The study of the impact of the experimental conditions is out the scope of this contribution. A detailed comment on this question will be added to the final manuscript.

- 5b should be represented in a SQ-SQ way to be more easily compared to Fig.5a.

It is a good idea. It will be done in the final manuscript.

- 6. Give the experimental details: such as the number of scan and recycling delays.

All NMR parameters (including NS and RD) are given in section 7 for all experiments/Figures.

Why not an indirect detection through ^1H ?

From our experience in natural abundance (0.14%!) ^{43}Ca MAS NMR spectroscopy, the rather short $T_1(^{43}\text{Ca})$'s are a clear advantage. It is why direct detection is usually performed.

In Figs.16b, the correlation of KS1 and KS2 resonances with the COM and COD decompositions is only a hypothesis.

Indeed. It leads to our conclusion that ^{43}Ca NMR has not to be used as a first tool of investigation for KS studies.

- 9-caption. The first sentence is not clear. Is the CPMAS spectrum also recorded under high-power ^1H decoupling?

Yes, it is. It will be specified in the final version.

- Part N° 7: sometimes $t_{90^\circ}(^1\text{H})$, sometimes $t_{90^\circ}(^1\text{H})$.

It will be carefully checked.

- Sx or Fig.Ax?

We will probably move to the Ax notation. I will ask the Editors about this point.

- Globally, most figures lack of experimental parameters.

See above my comment related to section 7.