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Open Access MAGNETIC RESONANCE Discussions

Interactive comment on "Open-source, 3D-printed, high-pressure (50 bar) liquid-nitrogen-cooled *para*-hydrogen generator" *by* Frowin Ellermann et al.

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Dear Igor Koptyug,

We thank you for your valuable comments which significantly improved our manuscript. We appreciate that you used the open discussion section of Magnetic Resonance journal. Hereby, we want to provide a point-by-point response to your post.

Your comment: "From the title, I had an impression that the generator or at least its essential parts were 3D-printed, which, as I found later, was not the case. I believe it may be a good idea to refine the paper title."

Answer: We understand that the title could be misleading and to avoid it the new title reads as "Open-source, partially 3D-printed, high-pressure (50 bar) liquid-nitrogen-cooled parahydrogen generator"

Your comment: "As always, I'm advocating the spelling of "parahydrogen" and "orthohydrogen" as single words without a dash, which I believe is the only correct way to spell them (cf. paratrooper, parabola, orthophosphoric acid; also in dictionaries, e.g.,https://www.thefreedictionary.com/parahydrogen)."

Answer: We understand your point and removed the dash. Additionally, we stick to the non-italic form.

"para-hydrogen" -> "parahydrogen" throughout the text

Your comment: "The word "allotrope" in the reference to parahydrogen is acceptable in the historic context, but in fact is incorrect. By definition, allotropy is the existence of a chemical element in two or more forms, which may differ in the arrangement of atoms in crystalline solids or in the occurrence of molecules that contain different numbers of atoms (e.g., graphite, charcoal, diamond, fullerenes). Parahydrogen is this not an allotropic form of H2 but rather its nuclear spinisomer."

Answer: We changed the word allotrope/allotropic to "nuclear spinisomer" except for the citation and the text referring to it.

Old text (e.g.): "The spin of hydrogen nuclei (proton) is the origin of the two allotropic forms or two spin isomers of hydrogen."

New text: "The spin of hydrogen nuclei (of protons) is the origin of the two nuclear spinisomer forms of dihydrogen."

Your comment: "line 40, naphthalene derivative (Stevanato et al., 2015) cannot be classified as spin isomer as it is not symmetric, so that the generalized Pauli principle is not applicable to it."

and

"Line 39, water (Mammoli et al., 2015; Meier et al., 2015) was not enriched in the Mammoli paper experiments, or at least could not be extracted to RT. A better reference to spin isomers of free water would be to the molecular beam separation experiments (e.g., doi: 10.1126/science.1200433 or 10.1021/acs.jpca.9b04294)."

Answer: We rephrased the sentences and added proposed references.

Old text (e.g.): "Hydrogen is not the only compound that has stable or long-lived spin isomers at room temperature (rt) there are many examples: deuterium (Knopp et al., 2003), water (Mammoli et al., 2015; Meier et al., 2015), ethylene (Zhivonitko et al., 2013), and even naphthalene derivative (Stevanato et al., 2015)."

New text: "Hydrogen is not the only compound that has stable or long-lived spinisomers at room temperature (rt) there are many examples: deuterium (Knopp et al., 2003), water (Kravchuk et al., 2011; Vermette et al., 2019) , ethylene (Zhivonitko et al., 2013) and methyl groups (Meier et al., 2013). Although some molecules are not symmetric and cannot be extracted at room temperature, they possess long-lived spin states of minutes (Pileio et al., 2008) and hours (Stevanato et al., 2015)."

Your comment: "There are a couple of very recent papers describing different parahydrogen gener-ator designs which the authors may wish to cite, doi: 10.1021/acs.analchem.0c03358doi: 10.1016/j.jmr.2020.106869"

Answer: These papers we not yet published when we finished our manuscript. Nevertheless, we included both generators to our overview table (Table 1). The updated table is attached to this comment.

We want to thank you again for sharing your thoughts in the open discussion. We picked this journal since we like the open access and open discussion approach.

With kind regards, Frowin Ellermann and Jan-Bernd Hövener

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Table 1: Performance comparison of several PHGs: (1) Bruker PHG 90, (2) dual-stage cryostats (DSC) (Hövener et al., 2013), (3) a pulsed PHG (Feng et al., 2012), (4) HyperSpin-PHG (Meier et al., 2019), (5) Automated PHG (Birchall et al., 2020), (6) He-dewar PHG (Du et al., 2020), (7) U-shape PHG (Kiryutin et al., 2017), (8) economical PHG (Jeong et al., 2018), (9) glass-trap PHG (Gamliel et al., 2010) and (10) in house designed and built PHG (this work). Given prices include all connectors, cylinders, and 19 % VAT. lN_2 stands for liquid nitrogen and "cc-He" for closed-cycle He compressor.

	Name	Operating temperature (K) [method]	f_{pH_2}(%)	Initial flow rate (SLM)	Max. pressure (bar)	Price (€)
1	Bruker BPHG 90	36-40 [cc-He]	85-92	≤ 0.2	10	100,000–150,000
2	DSC (Hövener et al., 2013)	25 [cc-He]	98 ± 2	4	50	37,000
3	Pulsed PHG (Feng et al., 2012)	15 [cc-He]	98	0.9	20	N.A.
4	HyperSpin-PHG (Meier et al., 2019)	20-77 [cc-He]	N.A.[a]	N.A.	Min. 10	N.A.
5	Automated PHG (Birchall et al., 2020)	40 [cc-He]	~87	0.15	33.8	<25,000
6	He-dewar PHG (Du et al., 2020)	30 [He]	97.3 ± 1.9	~0.3	4.5	N.A.
7	U-shape PHG (Kiryutin et al., 2017)	77 [lN_2]	~50	0.36[b]	Min. 3	N.A.
8	Economical PHG (Jeong et al., 2018)	77 [lN_2]	~50	N.A.	N.A.	N.A.
9	Glass-trap PHG (Gamliel et al., 2010)	77 [lN_2]	46.3 ± 1.3	0.0025[c]	~1	N.A.
10	This work	77 [lN_2]	51.6 ± 0.9	2.0[d]	50[e]	2,988[f]

Fig. 1.