Published in final edited form as:

ACS Earth Space Chem. 2020 April 16; 4(4): 495–498. doi:10.1021/acsearthspacechem.9b00326.

Parahydrogen-Induced Magnetization of Jovian Planets?

Eduard Y. Chekmenev*

Department of Chemistry, Integrative Biosciences (Ibio), Karmanos Cancer Institute (KCI), Wayne State University, Detroit, Michigan 48202, United States

Abstract

A long-overdue hypothesis on the origin of magnetic field of Jovian planets is presented. It is proposed that rapid parahydrogen $\leftrightarrow$ orthohydrogen exchange catalyzed by aerosol clouds of parahydrogen-rich planetary layers renders hyperpolarized nuclear spin state of orthohydrogen (and potentially other proton-containing compounds). This enhancement of nuclear spin polarization by several orders of magnitude (termed *hyperpolarization*) significantly enhances otherwise negligible proton magnetization. It is hypothesized that this persistent exchange process produces planetary magnetism on Jovian planets. This hypothesis builds on recent experimental evidence that parahydrogen exchange may indeed produce hyperpolarized orthohydrogen.

Keywords

parahydrogen; planetary magnetism; Jovian planet; hyperpolarization; nuclear spin; hydrogen; exchange; Uranus

All Jovian planets possess magnetic field, and their magnetic fields are so large that these fields dominate the weather of the planet, their moons and beyond ¹. Jupiter's magnetic moment is estimated to be approximately 20,000 times greater than that of the Earth. The existence of Jupiter's magnetic field was first predicted by the observations of a variable radio source ², and verified later by the Pioneer 10 space probe in 1973. The origin of a magnetic field of Jupiter and other Jovian planets remains unconfirmed to this day. Shortly after the discovery of magnetism of Jovian planets, the hypothesis of electrically conductive metallic hydrogen planetary core was introduced based on the prior theoretical predictions (*ca.* 1935) of metallic hydrogen modifications at ultra-high pressures ³. According to this theory the magnetic field of Jovian planets is created by the electric currents of the planetary metallic core composed of compressed hydrogen. Although several experimental studies have reported the creation of metallic hydrogen on a sub-second time scale ^{4–5}, these reports are disputed, and the experimental results have not been reproduced by other laboratories, thereby raising some concerns about the validity of the metallic hydrogen existence in Jovian planets.

*Corresponding Author: Eduard Y. Chekmenev Chekmenev@wayne.edu.

ASSOCIATED CONTENT

Supporting Information

The following files are available free of charge.

Computation of planetary magnetic moments due to nuclear spin polarization (PDF) Table S1 (PDF)

The lack of experimental validation is not the only challenge for the metallic hydrogen theory. Some smaller Jovian planets (*e.g.* Neptune and Uranus) cannot generate sufficiently high pressures to theoretically create the metallic hydrogen inside the planetary core. As a result of this fundamental theoretical gap, the variant of dynamo theory was proposed for smaller Jovian planets, where a combination of ammonia, methane and water is responsible for generating electrically conductive planetary layers^{1, 6}. However, to the best of my knowledge, there has been no experimental evidence for creating strong electrical conductivity in such mixtures. Moreover, any dynamo theories fall short of explaining the large tilt of the magnetic field axis with respect to the rotation axis of Neptune and Uranus by approximately 47° and 59° respectively¹. Furthermore, recent flybys' magnetic analysis of Jovian planets clearly shows very complex multi-polar (*i.e.* quadrupolar and octapolar) structure of magnetosphere of Neptune and Uranus^{7–8} and more recently of Jupiter^{9–10}, which is inconsistent with the expectation of a predominant dipolar structure predicted by the convectional planetary dynamo theory.

A magnetic field can be generally created in two ways. The moving electric charge is the first mechanism for inducing planetary magnetism. The second common source of the permanent magnetism is planetary components themselves. The key striking characteristic of all Jovian planets is their high content (90% or more) of hydrogen. Molecular dihydrogen dominates their upper planetary layers. Dihydrogen molecule exists in two spin isomer forms: parahydrogen (nuclear singlet, spin-0) and orthohydrogen (nuclear triplet, spin-1)¹¹. In the high-temperature limit, the equilibrium ratio of the two isomers is 1:3. Parahydrogen is the lower energy spin isomer. As a result, at low temperatures, the equilibrium shifts to the *para*-state. In 1986, Bowers and Weitekamp have demonstrated that the symmetry of the parahydrogen singlet can be revealed as large nuclear spin magnetization in the non-symmetric hydrogenation product of parahydrogen and unsaturated compounds through chemical symmetry breaking of parahydrogen nuclear singlet¹². As a result, nuclear spins gain a high degree of polarization, *i.e.* degree of alignment of nuclear spins. Consequently, these highly-polarized nuclear spin states are called *hyperpolarized*. The parahydrogen-derived nuclear spin polarization can reach the order of unity, and this highly magnetized non-equilibrium spin states are employed in NMR spectroscopy and MRI as a source of significant (by orders of magnitude) signal enhancement^{13–14}. This MR hyperpolarization technique has been called parahydrogen induced polarization or PHIP¹⁵, signifying that it is the NMR-silent parahydrogen state that can in fact serve as a source of massive nuclear spin hyperpolarization. In 2009, non-hydrogenative variant of PHIP has been introduced¹⁶. This relatively new technique (called Signal Amplification By Reversible Exchange or SABRE) employs parahydrogen exchange for nuclear spin hyperpolarization of small molecules¹⁶. Dihydrogen molecule is not chemically depleted in the SABRE exchange process – instead, it is released in the form of hyperpolarized orthohydrogen^{17–19}. This finding¹⁷ has no practical implications for the field of MRI and NMR applications yet, but can have immense implications for planetary science, because it shows that the interconversion of the two spin isomers (parahydrogen and orthohydrogen) can lead to production of hyperpolarized nuclear spins in orthohydrogen. Unlike parahydrogen (spin-0), orthohydrogen (spin-1) possesses net magnetic moment, and therefore hyperpolarized orthohydrogen molecules may produce large magnetization (especially on the planetary scale as discussed here) with the overall

value being the sum of all hyperpolarized dipoles. It should be made abundantly clear that proton spin polarization at thermodynamic equilibrium is negligible (and thus commonly discarded), *e.g.* less than 10^{-9} at the Earth's magnetic field (*ca.* 50 μT) and 77 K.

The spontaneous interconversion between orthohydrogen and parahydrogen is an extremely slow process, *i.e.* equilibration time for pure H_2 is $\sim 10^8$ seconds, because this is a forbidden transition¹¹. However, the interconversion process can be accelerated by a wide range of catalysts^{11, 13}. In all Jovian planets para-/orthohydrogen ratio is 1:3 in high temperature (>300 K) zones^{20–21} corresponding to thermodynamic nuclear spin polarization of protons¹³. In colder layers, catalysis by aerosols consisting of NH_3 , CH_4 , H_2S and other compounds renders para-/orthohydrogen ratio in accord to thermodynamic equilibrium²⁰, which otherwise (*i.e.* in the absence of such catalysis) would be close to that of high-temperature limit of 1:3 due to efficient mixing of colder and hot planetary zones on the time scale significantly shorter than spontaneous process of para-/orthohydrogen conversion²¹. Although departures from thermodynamic equilibrium of para-/orthohydrogen ratio exist in the Jovian planets²², the areas of thermodynamically equilibrated para-/orthohydrogen have been linked to ammonia-rich clouds^{20, 23} indicating that aerosol-based catalysis plays a crucial role in para-/orthohydrogen interconversion. Moreover, out of all Jovian planets, para-/orthohydrogen ratio of Uranus is the most thermodynamically equilibrated²⁴, and magnetosphere of Uranus is the most 'anomalous', *i.e.* (i) magnetic field axis has the largest tilt from rotation axis, (ii) the magnetic field at the equator ~ 23 μT is greater than that of two other heavier Jovian planets Saturn (~ 6.6 -fold greater mass) ~ 22 μT and Neptune (~ 1.2 -fold greater mass) ~ 13 μT respectively, (iii) the magnetic field has the highest asymmetry: *e.g.* ~ 10 μT strength at the South pole and ~ 110 μT at the North pole, etc.²⁵, indicating that fast interconversion of para- and orthohydrogen may be an important factor influencing magnetosphere of Jovian planets.

Here, it is hypothesized that these parahydrogen rich layers in the troposphere can undergo a sufficiently fast parahydrogen $\leftrightarrow$ orthohydrogen exchange process catalyzed by aerosols rendering a persistent existence of hyperpolarized proton nuclei in orthohydrogen (and potentially other more dilute proton-containing compounds). I note that although atmosphere of Jovian planets consists of many layers, it is troposphere, *i.e.*, the lower layer, that is important in the context of hyperpolarization process discussed here, because troposphere layers have low temperature—for example, Uranus troposphere (*ca.* 350 km thick) has temperature ranging from 50 K to 120 K—and troposphere of Jovian planets accounts for most of their atmospheric mass balance. Nuclear spin hyperpolarization of orthohydrogen protons is induced by cooling of dihydrogen gas, which forms parahydrogen rich mixture acting as the fundamental source of hyperpolarization, Figure 1. The excess of parahydrogen at low temperature (well above thermodynamic 1:3 equilibrium distribution at high temperature limit, Figure 2b) leads to production of hyperpolarized orthohydrogen, Figure 2a. Hyperpolarization of orthohydrogen protons leads to enhanced net magnetization which generates a fraction or the entire static magnetism of Jovian planets. Note that nuclear spin relaxation may lead to depolarization of hyperpolarized orthohydrogen to thermally polarized hydrogen, and the corresponding relaxation rate (k_3) must not be significantly larger than the back-conversion rate (k_2) of orthohydrogen to parahydrogen, Figure 2a. In other words, the parahydrogen $\leftrightarrow$ orthohydrogen exchange rate must be significantly greater

than the relaxation rate of the hyperpolarized state. Although it is parahydrogen singlet state that provides the source of nuclear spin polarization in this model, parahydrogen itself is not magnetized, and it is hyperpolarized orthohydrogen that acts as a carrier of magnetization. As a result, the maximum fractional magnetization dependence on temperature (Figure 2c) exhibits a clear maximum at ~63 K. The quantity of dihydrogen in all Jovian planets is certainly large enough to generate sufficient quantity of hyperpolarized protons to account for a fraction or the entire planetary magnetism (see Supporting Information for details).

The key strength of the proposed hypothesis is the possibility to explain the complex magnetic field structure of Jovian planets, because it is likely modulated by the heterogeneously distributed catalytic aerosols. Unlike many other theories, the proposed hypothesis can be potentially readily tested by probing the troposphere of a Jovian planet by NMR spectroscopy during future flyby missions.

The described here hypothesis will clearly benefit from future quantitative modelling, which will likely require the development of new kind of nuclear magnetic spin physics to describe nuclear spin dynamics on the planetary scale.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

ACKNOWLEDGMENT

The author thanks NSF under Grants CHE-1836308 and CHE-1904780, National Cancer Institute under 1R21CA220137 and 1U01CA202229, DOD CDMRP under W81XWH-12-1-0159/BC112431 and W81XWH-15-1-0271 for funding sources. The author thanks Dr. Panayiotis Nikolaou for proof-reading the manuscript.

REFERENCES

1. Kivelson MG; Bagenal F, Planetary Magnetospheres. In Encyclopedia of the Solar System, McFadden L-A; Johnson T; Weissman P, Eds. Academic Press: 2007; pp 519–540.
2. Burke BF; Franklin KL, Observations of a variable radio source associated with the planet Jupiter. J. Geophys. Res. 1955, 60 (2), 213–217.
3. Wigner E; Huntington HB, On the Possibility of a Metallic Modification of Hydrogen. J. Chem. Phys. 1935, 3 (12), 764–770.
4. Dias RP; Silvera IF, Observation of the Wigner-Huntington transition to metallic hydrogen. Science2017, 355 (6326), 715–718. [PubMed: 28126728]
5. Zaghou M; Salamat A; Silvera IF, Evidence of a first-order phase transition to metallic hydrogen. Phys. Rev. B2016, 93 (15), 155128.
6. Stanley S; Bloxham J, Convective-region geometry as the cause of Uranus' and Neptune's unusual magnetic fields. Nature2004, 428 (6979), 151–153. [PubMed: 15014493]
7. Stanley S; Bloxham J, Numerical dynamo models of Uranus' and Neptune's magnetic fields. Icarus2006, 184 (2), 556–572.
8. Stanley S; Bloxham J, On the secular variation of Saturn's magnetic field. Phys. Earth Planet. In. 2016, 250, 31–34.
9. Moore KM; Yadav RK; Kulowski L; Cao H; Bloxham J; Connerney JEP; Kotsiaros S; Jørgensen JL; Merayo JMG; Stevenson DJ; Bolton SJ; Levin SM, A complex dynamo inferred from the hemispheric dichotomy of Jupiter's magnetic field. Nature2018, 561 (7721), 76–78. [PubMed: 30185957]

10. Connerney JEP; Adriani A; Allegrini F; Bagenal F; Bolton SJ; Bonfond B; Cowley SWH; Gerard J-C; Gladstone GR; Grodent D; Hospodarsky G; Jorgensen JL; Kurth WS; Levin SM; Mauk B; McComas DJ; Mura A; Paranicas C; Smith EJ; Thorne RM; Valek P; Waite J, Jupiter's magnetosphere and aurorae observed by the Juno spacecraft during its first polar orbits. *Science* 2017, 356 (6340), 826–832. [PubMed: 28546207]
11. Farkas A, Orthohydrogen, Parahydrogen, and Heavy Hydrogen. Cambridge University Press: Cambridge, 1935.
12. Bowers CR; Weitekamp DP, Transformation of Symmetrization Order to Nuclear-Spin Magnetization by Chemical-Reaction and Nuclear-Magnetic-Resonance. *Phys. Rev. Lett.* 1986, 57 (21), 2645–2648. [PubMed: 10033824]
13. Hövener J-B; Pravdivtsev AN; Kidd B; Bowers CR; Glöggler S; Kovtunov KV; Plaumann M; Katz-Brull R; Buckenmaier K; Jerschow A; Reineri F; Theis T; Shchepin RV; Wagner S; Bhattacharya P; Zacharias NM; Chekmenev EY, Parahydrogen-based Hyperpolarization for Biomedicine. *Angew. Chem. Int. Ed.* 2018, 57 (35), 11140–11162.
14. Golman K; Axelsson O; Johannesson H; Mansson S; Olofsson C; Petersson JS, Parahydrogen-induced polarization in imaging: Subsecond C-13 angiography. *Magn. Reson. Med.* 2001, 46 (1), 1–5. [PubMed: 11443703]
15. Eisenschmid TC; Kirss RU; Deutsch PP; Hommeltoft SI; Eisenberg R; Bargon J; Lawler RG; Balch AL, Para Hydrogen Induced Polarization In Hydrogenation Reactions. *J. Am. Chem. Soc.* 1987, 109 (26), 8089–8091.
16. Adams RW; Aguilar JA; Atkinson KD; Cowley MJ; Elliott PIP; Duckett SB; Green GGR; Khazal IG; Lopez-Serrano J; Williamson DC, Reversible Interactions with para-Hydrogen Enhance NMR Sensitivity by Polarization Transfer. *Science* 2009, 323 (5922), 1708–1711. [PubMed: 19325111]
17. Barskiy DA; Kovtunov KV; Koptug IV; He P; Groome KA; Best QA; Shi F; Goodson BM; Shchepin RV; Coffey AM; Waddell KW; Chekmenev EY, The feasibility of formation and kinetics of NMR Signal Amplification by Reversible Exchange (SABRE) at high magnetic field (9.4 T). *J. Am. Chem. Soc.* 2014, 136 (9), 3322–3325. [PubMed: 24528143]
18. Glogler S; Muller R; Colell J; Emondts M; Dabrowski M; Blumich B; Appelt S, Para-hydrogen induced polarization of amino acids, peptides and deuterium-hydrogen gas. *Phys. Chem. Chem. Phys.* 2011, 13 (30), 13759–13764. [PubMed: 21720644]
19. Truong ML; Theis T; Coffey AM; Shchepin RV; Waddell KW; Shi F; Goodson BM; Warren WS; Chekmenev EY, ¹⁵N Hyperpolarization By Reversible Exchange Using SABRE-SHEATH. *J. Phys. Chem. C* 2015, 119 (16), 8786–8797.
20. Massie ST; Hunten DM, Conversion of para and ortho hydrogen in the Jovian planets. *Icarus* 1982, 49 (2), 213–226.
21. Smith WH, On the ortho-para equilibrium of H₂ in the atmospheres of the Jovian planets. *Icarus* 1978, 33 (1), 210–216.
22. Conrath BJ; Gierasch PJ; Ustinov EA, Thermal Structure and Para Hydrogen Fraction on the Outer Planets from Voyager IRIS Measurements. *Icarus* 1998, 135 (2), 501–517.
23. Carlson BE; Lacis AA; Rossow WB, Ortho-para-hydrogen Equilibration on Jupiter. *Astrophys. J.* 1992, 393 (1), 357–372.
24. Fouchet T; Lellouch E; Feuchtgruber H, The hydrogen ortho-to-para ratio in the stratospheres of the giant planets. *Icarus* 2003, 161 (1), 127–143.
25. Ness NF; Acuna MH; Behannon KW; Burlaga LF; Connerney JEP; Lepping RP; Neubauer FM, Magnetic Fields at Uranus. *Science* 1986, 233 (4759), 85–89. [PubMed: 17812894]

Figure 1.

The overall schematic of dihydrogen nuclear spin polarization. High-temperature (>300 K) zone exhibit high-temperature thermodynamic distribution of para- and orthohydrogen (1:3) corresponding to thermodynamic nuclear spin polarization of protons, *i.e.* $<10^{-9}$.¹³ In the colder zone in troposphere layers, chemical exchange between para- and orthohydrogen (on aerosol clouds) results in (i) thermodynamic equilibrium of para-/orthohydrogen ratio (corresponding to parahydrogen-rich condition, *e.g.*, 50% para- at 77 K), and (ii) non-thermodynamic nuclear spin polarization of orthohydrogen corresponding to hyperpolarized nuclear spin state of orthohydrogen.¹⁷

Figure 2.

a) The schematic of dihydrogen transformation due to rapid parahydrogen $\leftrightarrow$ orthohydrogen exchange process catalyzed by aerosols and nuclear spin relaxation. Hyperpolarized orthohydrogen is created due to spin conversion from parahydrogen. The produced hyperpolarized state may undergo relaxation process resulting in parahydrogen-induced magnetization depletion. The corresponding relaxation rate (k_3) of hyperpolarized state must not be significantly greater than the rate of orthohydrogen conversion to parahydrogen (k_2), otherwise the level of parahydrogen-induced magnetization will be significantly reduced. b) Equilibrium parahydrogen percentage fraction (χ) as a function of temperature. c) maximum fractional parahydrogen-induced magnetization (defined as $(\chi - 25\%)(100\% - \chi)/75\%/100\%$) as a function of temperature under conditions of $k_3 \ll k_2$.