

1. Published international peer reviewed papers

1. S. Leppävuori, J. Levoska, **J. Vaara**, and O. Kusmartseva: *Laser ablation deposition of diamond-like carbon films*, Materials Research Society Symposium Proceedings Vol. **285**, 557–562 (1993).
2. **J. Vaara**, J. Jokisaari, T. T. Rantala, and J. Lounila: *Computational and experimental study of NMR relaxation of quadrupolar noble gas nuclei in organic solvents*, Molecular Physics **82**, 13–27 (1994).
3. Tapio T. Rantala, Tuomo S. Rantala, Vilho Lantto, and **Juha Vaara**: *Surface reconstruction of the (10 $\bar{1}$ 0) face of wurtzite CdS*, Surface Science **352–354**, 77–82 (1996).
4. Marja Hyvönen, Mika Ala-Korpela, **Juha Vaara**, Tapio T. Rantala, and Jukka Jokisaari: *Effects of two double bonds on the hydrocarbon interior of a phospholipid bilayer*, Chemical Physics Letters **246**, 300–306 (1995).
5. **Juha Vaara**, Kari Oikarinen, Jukka Jokisaari, and Juhani Lounila: *Anisotropy of ^1H and ^{13}C shielding tensors in chloroform*, Chemical Physics Letters **253**, 340–348 (1996).
6. J.-H. Kantola, **J. Vaara**, T. T. Rantala, and J. Jokisaari: *Molecular dynamics simulations for Xe absorbed in zeolites*, Materials Research Society Symposium Proceedings Vol. **408**, 599–604 (1996).
7. Jaakko Kaski, **Juha Vaara**, and Jukka Jokisaari: *^{13}C - ^{13}C spin-spin coupling tensors in benzene as determined experimentally by liquid crystal NMR and theoretically by *ab initio* calculations*, Journal of the American Chemical Society **118**, 8879–8886 (1996).
8. Tuomas Koskela, Mika Ylihautala, **Juha Vaara**, and Jukka Jokisaari: *^{13}C NMR spectroscopy of methane adsorbed in SAPO-11 molecular sieve*, Chemical Physics Letters **261**, 425–430 (1996).
9. Marja Hyvönen, Mika Ala-Korpela, **Juha Vaara**, Tapio T. Rantala, and Jukka Jokisaari: *Inequivalence of single CH_a and CH_b methylene bonds in the interior of a diunsaturated lipid bilayer from a molecular dynamics simulation*, Chemical Physics Letters **268**, 55–60 (1997).

10. Mika Ylihautala, **Juha Vaara**, Petri Ingman, Jukka Jokisaari, and Peter Diehl: ^{14}N and ^2H NMR study of the mesophases of CTAB in formamide, *Journal of Physical Chemistry B* **101**, 32–38 (1997).
11. Juhani Lounila, **Juha Vaara**, Yrjö Hiltunen, Anja Pulkkinen, Jukka Jokisaari, Mika Ala-Korpela, and Kenneth Ruud: *Isotope and temperature effects on the ^{13}C and ^{77}Se nuclear shielding in carbon diselenide*, *Journal of Chemical Physics* **107**, 1350–1361 (1997).
12. **Juha Vaara**, Jaakko Kaski, Jukka Jokisaari, and Peter Diehl: *NMR properties of formamide: A first principles and experimental study*, *Journal of Physical Chemistry A* **101**, 5069–5081 (1997), *Ibid.* A **101**, 9185 (1997).
13. **Juha Vaara** and Yrjö Hiltunen: *Deuterium quadrupole coupling tensors in methyl halides: Ab initio effective core potential and liquid crystal nuclear magnetic resonance study*, *Journal of Chemical Physics* **107**, 1744–1752 (1997).
14. Juha-Heikki Kantola, **Juha Vaara**, Tapio T. Rantala, and Jukka Jokisaari: ^{129}Xe adsorbed in AlPO_4 -11 molecular sieve: *A molecular dynamics simulation of adsorbate dynamics and NMR chemical shift*, *Journal of Chemical Physics* **107**, 6470–6478 (1997).
15. Jaakko Kaski, Perttu Lantto, **Juha Vaara**, and Jukka Jokisaari: *Experimental and theoretical ab initio study of the ^{13}C - ^{13}C spin-spin coupling and ^1H and ^{13}C shielding tensors in ethane, ethene and ethyne*, *Journal of the American Chemical Society* **120**, 3993–4005 (1998).
16. **Juha Vaara**, Kenneth Ruud, Olav Vahtras, Hans Ågren, and Jukka Jokisaari: *Quadratic response calculation of the electronic spin-orbit contribution to nuclear shielding tensors*, *Journal of Chemical Physics* **109**, 1212–1222 (1998).
17. Boris Minaev, **Juha Vaara**, Kenneth Ruud, Olav Vahtras, and Hans Ågren: *Internuclear distance dependence of the spin-orbit coupling contributions to proton NMR chemical shifts*, *Chemical Physics Letters* **295**, 455–461 (1998).
18. Karol Jackowski, Michał Jaszucki, Włodzimierz Makulski, and **Juha Vaara**: *Rovibrationally averaged nuclear shielding constants in OCS*, *Journal of Magnetic Resonance* **135**, 444–453 (1998).
19. **Juha Vaara**, Juhani Lounila, and Jukka Jokisaari: *Comment to: Nematic mixture methods for the determination of chemical shift anisotropy*, *Chemical Physics Letters* **296**, 541–544 (1998).

20. Tuomas Koskela, Mika Ylihautala, Jukka Jokisaari, and **Juha Vaara**: ^{13}C NMR of methane in $\text{AlPO}_4\text{-11}$ molecular sieve: exchange effects and shielding anisotropy, *Physical Review B* **58**, 14833–14836 (1998).
21. **Juha Vaara**, Juhani Lounila, Kenneth Ruud, and Trygve Helgaker: *Rovibrational effects, temperature dependence, and isotope effects on the nuclear shielding tensors of water: a new ^{17}O absolute shielding scale*, *Journal of Chemical Physics* **109**, 8388–8397 (1998).
22. Kenneth Ruud, **Juha Vaara**, Juhani Lounila, and Trygve Helgaker: *Vibrationally averaged magnetizabilities and rotational \mathbf{g} -tensors of the water molecule*, *Chemical Physics Letters* **297**, 467–474 (1998).
23. **Juha Vaara**, Jaakko Kaski, and Jukka Jokisaari: *Indirect fluorine coupling anisotropies in p -difluorobenzene: Implications to orientation and structure determination of fluorinated liquid crystals*, *Journal of Physical Chemistry A* **103**, 5675–5684 (1999).
24. **Juha Vaara**, Kenneth Ruud, and Olav Vahtras: *Second- and third-order spin-orbit contributions to nuclear shielding tensors*, *Journal of Chemical Physics* **111**, 2900–2909 (1999).
25. **Juha Vaara**, Kenneth Ruud, and Olav Vahtras: *Correlated response calculations of the spin-orbit interaction contribution to nuclear spin-spin couplings*, *Journal of Computational Chemistry* **20**, 1314–1327 (1999).
26. Jaakko Kaski, Perttu Lantto, Tapio Rantala, Jyrki Schroderus, **Juha Vaara**, and Jukka Jokisaari: *Experimental and theoretical study of the spin-spin coupling tensors in methylsilane*, *Journal of Physical Chemistry A* **103**, 9669–9677 (1999).
27. Perttu Lantto, Jaakko Kaski, **Juha Vaara**, and Jukka Jokisaari: *Spin-spin coupling tensors in fluoromethanes*, *Chemistry-A European Journal* **6**, 1395–1406 (2000).
28. Olga L. Malkina, **Juha Vaara**, Bernd Schimmelpfennig, Marketá Munzarová, Vladimir G. Malkin, and Martin Kaupp: *Density functional calculations of electronic g -tensors using spin-orbit pseudopotentials and mean-field all-electron spin-orbit operators*, *Journal of the American Chemical Society* **122**, 9206–9218 (2000).

29. **Juha Vaara**, Olga L. Malkina, Hermann Stoll, Vladimir G. Malkin, and Martin Kaupp: *Study of relativistic effects on nuclear shieldings using density-functional theory and spin-orbit pseudopotentials*, Journal of Chemical Physics **114**, 61–71 (2001).
30. Marja T. Hyvönen, Yrjö Hiltunen, Wael El-Deredy, Timo Ojala, **Juha Vaara**, Petri T. Kovanen, and Mika Ala-Korpela: *Application of self-organising maps in conformational analysis of lipids*, Journal of the American Chemical Society **123**, 810–816 (2001).
31. Perttu Lantto and **Juha Vaara**: *Effect of correlating core orbitals in calculations of nuclear spin-spin couplings*, Journal of Chemical Physics **114**, 5482–5490 (2001).
32. **Juha Vaara** and Pekka Pyykkö: *Magnetic-field-induced quadrupole splitting in gaseous and liquid ^{131}Xe NMR: Quadratic and quartic field dependence*, Physical Review Letters **86**, 3268–3271 (2001).
33. Martin Kaupp, Christian Remenyi, **Juha Vaara**, Olga L. Malkina, and Vladimir G. Malkin: *Density functional calculations of electronic g -tensors for semiquinone radical anions. The role of hydrogen bonding and substituent effects*, Journal of the American Chemical Society **124**, 2709–2722 (2002).
34. Perttu Lantto, **Juha Vaara**, Anu Kantola, Ville-Veikko Telkki, Bernd Schimmelpfennig, Kenneth Ruud, and Jukka Jokisaari: *Relativistic spin-orbit coupling effects on secondary isotope shifts of ^{13}C nuclear shielding in CX_2 (X = O, S, Se, Te)*, Journal of the American Chemical Society **124**, 2762–2771 (2002).
35. Perttu Lantto, **Juha Vaara**, and Trygve Helgaker: *Spin-spin coupling tensors by the density-functional linear response theory*, Journal of Chemical Physics **117**, 5998–6009 (2002).
36. Maria Engström, **Juha Vaara**, Bernd Schimmelpfennig, and Hans Ågren: *Density functional theory calculations of EPR parameters of a nitroxide spin label in Tissue factor and Factor VIIa protein complex*, Journal of Physical Chemistry B **106**, 12354–12360 (2002).
37. **Juha Vaara**, Jukka Jokisaari, Roderick E. Wasylishen, and David L. Bryce: *Spin-spin coupling tensors as determined by experiment and computational*

- chemistry*, Progress in Nuclear Magnetic Resonance Spectroscopy **41**, 233–304 (2002).
38. Zilvinas Rinkevicius, **Juha Vaara**, Lyudmyla Telyatnyk, and Olav Vahtras: *Calculations of nuclear magnetic shielding in paramagnetic molecules*, Journal of Chemical Physics **118**, 2550–2561 (2003).
 39. **Juha Vaara** and Pekka Pyykkö: *Relativistic, nearly basis-set-limit nuclear magnetic shielding constants of the rare gases He–Rn: A way to absolute NMR shielding scales*, Journal of Chemical Physics **118**, 2973–2976 (2003).
 40. **Juha Vaara**, Pekka Manninen, and Juhani Lounila: *Magnetic field dependence of nuclear magnetic shielding in closed-shell atomic systems*, Chemical Physics Letters **372**, 750–757 (2003).
 41. Pekka Manninen, Perttu Lantto, **Juha Vaara**, and Kenneth Ruud: *Perturbational ab initio calculations of relativistic contributions to nuclear magnetic resonance shielding tensors*, Journal of Chemical Physics **119**, 2623–2637 (2003).
 42. **Juha Vaara**, Pekka Manninen, and Perttu Lantto: *Perturbational and ECP calculation of relativistic effects in NMR shielding and spin-spin coupling*, in M. Kaupp, M. Bühl, and V. G. Malkin (eds.), *Calculation of NMR and EPR Parameters: Theory and Applications* (Wiley-VCH, Weinheim, 2004), pp. 209–226.
 43. Lyudmyla Telyatnyk, **Juha Vaara**, Zilvinas Rinkevicius, and Olav Vahtras: *Influence of hydrogen bonding in the paramagnetic NMR shieldings of nitronyl-nitroxide derivative molecules*, Journal of Physical Chemistry B **108**, 1197–1206 (2004).
 44. Pekka Manninen and **Juha Vaara**: *Magnetic-field dependence of ^{59}Co nuclear magnetic shielding in Co(III) complexes*, Physical Review A **69**, 022503 (2004).
 45. Alexei Arbuznikov, **Juha Vaara**, and Martin Kaupp: *Relativistic spin-orbit effects on hyperfine coupling tensors by density-functional theory*, Journal of Chemical Physics **120**, 2127–2139 (2004).
 46. Pekka Manninen, **Juha Vaara**, and Kenneth Ruud: *Perturbational relativistic theory of electron spin resonance g-tensor*, Journal of Chemical Physics **121**, 1258–1265 (2004).

47. Mikael P. Johansson, Dage Sundholm, and **Juha Vaara**: *Au₃₂: A 24-carat golden fullerene*, *Angewandte Chemie International Edition* **43**, 2678–2681 (2004); *Angewandte Chemie* **116**, 2732–2735 (2004).
48. Christian Remenyi, Roman Reviakine, Alexei V. Arbuznikov, **Juha Vaara**, and Martin Kaupp: *Spin-orbit effects on hyperfine coupling tensors in transition metal complexes using hybrid density functionals and accurate spin-orbit operators*, *Journal of Physical Chemistry A* **108**, 5026–5033 (2004).
49. Teemu S. Pennanen, **Juha Vaara**, Perttu Lantto, Atte J. Sillanpää, Kari Laasonen, and Jukka Jokisaari: *Nuclear magnetic shielding and quadrupole coupling tensors in liquid water: A combined molecular dynamics simulation and quantum chemical study*, *Journal of the American Chemical Society* **126**, 11093–11102 (2004).
50. Pekka Manninen, **Juha Vaara**, and Pekka Pyykkö: *Magnetic field-induced quadrupole coupling in the nuclear magnetic resonance of noble gas atoms and molecules*, *Physical Review A* **70**, 043401–043409 (2004).
51. Rodolfo H. Romero and **Juha Vaara**: *Laser-induced splittings in the nuclear magnetic resonance spectra of the rare gas atoms*, *Chemical Physics Letters* **400**, 226–230 (2004).
52. Matti Hanni, Perttu Lantto, Nino Runeberg, Jukka Jokisaari, and **Juha Vaara**: *Calculation of binary magnetic properties and potential energy curve in xenon dimer: Second virial coefficient of ¹²⁹Xe nuclear shielding*, *Journal of Chemical Physics* **121**, 5908–5919 (2004).
53. Pekka Manninen, Kenneth Ruud, Perttu Lantto, and **Juha Vaara**: *Leading-order relativistic effects on nuclear magnetic resonance shielding tensors*, *Journal of Chemical Physics* **122**, 114107:1–8 (2005), *Ibid.* **124**, 149901:1–2 (2006).
54. Ville Weijo, Pekka Manninen, and **Juha Vaara**: *Perturbational calculations of parity-violating effects in nuclear magnetic resonance parameters*, *Journal of Chemical Physics* **123**, 054501:1–8 (2005).
55. Teemu O. Pennanen and **Juha Vaara**: *Density-functional calculations of relativistic spin-orbit effects on nuclear magnetic shielding in paramagnetic molecules*, *Journal of Chemical Physics* **123**, 174102:1–10 (2005).

56. Pekka Manninen and **Juha Vaara**: *Systematic Gaussian basis-set limit using completeness-optimized primitive sets. A case for magnetic properties*, Journal of Computational Chemistry **27**, 434–445 (2006).
57. Pekka Manninen and **Juha Vaara**: *Comment on Calculation of nuclear magnetic shieldings using an analytically differentiated relativistic shielding formula*, Journal of Chemical Physics **124**, 137101:1–2 (2006).
58. Perttu Lantto, Rodolfo H. Romero, Sergio S. Gómez, Gustavo A. Aucar and **Juha Vaara**: *Relativistic heavy-atom effects on heavy-atom nuclear shieldings*, Journal of Chemical Physics **125**, 184113:1–13 (2006).
59. Teemu S. Pennanen, Perttu Lantto, Atte J. Sillanpää and **Juha Vaara**: *Nuclear magnetic resonance chemical shifts and quadrupole couplings for different hydrogen-bonding cases occurring in liquid water: A computational study*, Journal of Physical Chemistry A **111**, 182–192 (2007).
60. Michal Straka and **Juha Vaara**: *Density functional calculations of ^3He chemical shift in endohedral helium fullerenes: Neutral, anionic and di-helium species*, Journal of Physical Chemistry A **110**, 12338–12341 (2006).
61. Perttu Lantto and **Juha Vaara**: *Calculations of quadrupole couplings in noble gas–noble metal fluorides: Interplay of relativistic and electron correlation effects*, Journal of Chemical Physics **125**, 174315:1–7 (2006).
62. Anu M. Kantola, Susanna Ahola, **Juha Vaara**, Jani Saunavaara and Jukka Jokisaari: *Experimental and quantum-chemical determination of the ^2H quadrupole coupling tensor in deuterated benzenes*, Physical Chemistry Chemical Physics **9**, 481–490 (2007).
63. Juho Lintuvuori, Michal Straka, and **Juha Vaara**: *Nuclear magnetic resonance parameters of atomic xenon dissolved in Gay-Berne model liquid crystal*, Physical Review E **75**, 031707:1–13 (2007).
64. Ville Weijo, Radovan Bast, Pekka Manninen, Trond Saue, and **Juha Vaara**: *Methodological aspects in the calculation of parity-violating effects in nuclear magnetic resonance parameters*, Journal of Chemical Physics **126**, 074107:1–10 (2007).
65. Pekka Pyykkö, Cong Wang, Michal Straka, and **Juha Vaara**: *A London-type formula for the dispersion interactions of endohedral A@B systems*, Physical Chemistry Chemical Physics **9**, 2954–2958 (2007).

66. **Juha Vaara:** *Theory and computation of nuclear magnetic resonance parameters*, Physical Chemistry Chemical Physics **9**, 5399–5418 (2007).
67. Perttu Lantto and **Juha Vaara:** ^{129}Xe *chemical shift by the perturbational relativistic method: Xenon fluorides*, Journal of Chemical Physics **127**, 084312:1–9 (2007).
68. Matti Hanni, Perttu Lantto, Miroslav Iliáš, Hans Joergen Aagaard Jensen, and **Juha Vaara:** *Relativistic effects in the intermolecular interaction-induced nuclear magnetic resonance parameters of xenon dimer*, Journal of Chemical Physics **127**, 164313:1–13 (2007).
69. Michal Straka, Perttu Lantto, Markku Räsänen, and **Juha Vaara:** *Theoretical predictions of nuclear magnetic resonance parameters in a novel organo-xenon species. Chemical shifts and nuclear quadrupole couplings in HXeCCH*, Journal of Chemical Physics **127**, 234314:1–13 (2007).
70. Ville Weiho, Pekka Manninen, and **Juha Vaara:** *Effect of molecular size on the parity-non-conserving contributions to the nuclear magnetic resonance shielding constant*, Theoretical Chemistry Accounts **121**, 53–57 (2008).
71. Michal Straka, Perttu Lantto, and **Juha Vaara:** *Toward calculations of the ^{129}Xe chemical shift in $\text{Xe}@C_{60}$ at experimental conditions: Relativity, correlation, and dynamics*, Journal of Physical Chemistry A **112**, 2658–2668 (2008).
72. Stefan Taubert, Michal Straka, Teemu O. Pennanen, Dage Sundholm, and **Juha Vaara:** *Dynamics and magnetic resonance properties of $\text{Sc}_3\text{C}_2@C_{80}$ and its monoanion*, Physical Chemistry Chemical Physics **10**, 7158–7168 (2008).
73. Teemu O. Pennanen and **Juha Vaara:** *Nuclear magnetic resonance chemical shift in an arbitrary electronic spin state*, Physical Review Letters **100**, 133002:1–4 (2008).
74. M. Hakala, K. Nygård, **J. Vaara**, M. Itou, Y. Sakurai, and K. Hämäläinen: *Charge localization in alcohol isomers studied by Compton scattering*, Journal of Chemical Physics **130**, 034506:1–8 (2009).
75. Suvi Ikäläinen, Perttu Lantto, Pekka Manninen, and **Juha Vaara:** *Laser-induced nuclear magnetic resonance splitting in hydrocarbons*, Journal of Chemical Physics **129**, 124102:1–8 (2008); Virtual Journal of Nanoscale Science

and Technology, October 6, 2008; Virtual Journal of Ultrafast Science, October (2008).

76. Mikael P. Johansson, **Juha Vaara**, and Dage Sundholm: *Exploring the stability of golden fullerenes*, Journal of Physical Chemistry C **112**, 19311–19315 (2008).
77. Matti Hanni, Perttu Lantto, and **Juha Vaara**: *Pairwise additivity in the nuclear magnetic resonance interactions of atomic xenon*, Physical Chemistry Chemical Physics **11**, 2485–2496 (2009).
78. Helmi Liimatainen, Teemu O. Pennanen, and **Juha Vaara**: *^1H chemical shifts in non-axial, paramagnetic chromium(III) complexes: Application of novel $p\text{NMR}$ shift theory*, Canadian Journal of Chemistry **87**, 954–964 (2009).
79. Michał Jaszuński and **Juha Vaara**: *^{19}F spin-spin coupling in peri-difluoronaphthalene*, Physical Chemistry Chemical Physics **11**, 4136–4140 (2009).
80. Marja Hyvärinen, **Juha Vaara**, Anna Goldammer, Barbara Kutzky, Kaspar Hegetschweiler, Martin Kaupp, and Michal Straka: *Characteristic spin-orbit induced $^1\text{H}(\text{CH}_2)$ chemical shifts upon deprotonation of group 9 polyamine aqua and alcohol complexes*, Journal of the American Chemical Society **131**, 11909–11918 (2009).
81. Teemu O. Pennanen, Jan Macháček, Stefan Taubert, **Juha Vaara**, and Drahomir Hnyk: *Ferrocene-like iron bis(dicarbollide), $[\text{3-Fe}^{\text{III}}-(1,2\text{-C}_2\text{B}_9\text{H}_{11})_2]^-$. The first experimental and theoretical refinement of a paramagnetic ^{11}B NMR spectrum*, Physical Chemistry Chemical Physics **12**, 7018–7025 (2010).
82. Suvi Ikäläinen, Perttu Lantto, Pekka Manninen, and **Juha Vaara**: *NMR tensors in planar hydrocarbons of increasing size*, Physical Chemistry Chemical Physics **11**, 11404–11414 (2009).
83. Nergiz Özcan, Tommi Kortelainen, Vyacheslav Golovanov, Tapio T. Rantala, and **Juha Vaara**: *Electron spin resonance parameters of bulk oxygen vacancy in semiconducting tin dioxide*, Physical Review B **81**, 235202:1–10 (2010).
84. Stanislav Standara, Kateřina Maliňáková, Radek Marek, Jaromír Marek, Michal Hocek, **Juha Vaara**, and Michal Straka: *Understanding the NMR chemical shifts for 6-halopurines: Role of structure, solvent and relativistic effects*, Physical Chemistry Chemical Physics **12**, 5126–5139 (2010).

85. Anu M. Kantola, Perttu Lantto, **Juha Vaara**, and Jukka Jokisaari: *Carbon and proton shielding tensors in methyl halides*, Physical Chemistry Chemical Physics **12**, 2679–2692 (2010).
86. Teemu S. Pennanen, Perttu Lantto, Mikko Hakala, and **Juha Vaara**: *Nuclear magnetic resonance parameters in water dimer*, Theoretical Chemistry Accounts **129**, 313–324 (2011).
87. Suvi Ikäläinen, Michael V. Romalis, Perttu Lantto, and **Juha Vaara**: *Chemical distinction by nuclear spin optical rotation*, Physical Review Letters **105**, 153001:1–4 (2010).
88. Matti Hanni, Perttu Lantto, and **Juha Vaara**: *Nuclear spin relaxation due to chemical shift anisotropy of gas-phase ^{129}Xe* , Physical Chemistry Chemical Physics **13**, 13704–13708 (2011)
89. J. Lehtola, M. Hakala, **J. Vaara**, and K. Hämäläinen: *Calculation of isotropic Compton profiles with Gaussian basis sets*, Physical Chemistry Chemical Physics **13**, 5630–5641 (2011).

2. International peer-reviewed papers in press

90. Jiří Mareš, Helmi Liimatainen, Kari Laasonen, and **Juha Vaara**: *Solvation structure and dynamics of $\text{Ni}^{2+}(\text{aq})$ from first principles*, Journal of Chemical Theory and Computation, *in press*.
91. Jiří Mareš, Helmi Liimatainen, Teemu O. Pennanen, and **Juha Vaara**: *Magnetic properties of $\text{Ni}^{2+}(\text{aq})$ from first principles*, Journal of Chemical Theory and Computation, *in press*.

3. Submitted papers

92. Juho Roukala, Alejandro F. Maldonado, **Juha Vaara**, Gustavo A. Aucar, and Perttu Lantto: *Metal chemical shifts in model compounds of group-12 elements*, submitted for publication in Physical Chemistry Chemical Physics.

4. Talks at international conferences

Invited

1. **Juha Vaara**, Pekka Manninen, Perttu Lantto, and Kenneth Ruud: *Relativistic effects on magnetic resonance parameters by perturbation theory*, invited talk on Coastal Voyage in Quantum Chemistry, Tromsø-Trondheim, Norway, September 18–21, 2003.
2. **Juha Vaara**: *Magnetic and laser field effects on NMR parameters*, invited talk in Molecular Modeling Meeting, KTH Stockholm, May 26–28, 2004.
3. **Juha Vaara**, Teemu S. Pennanen, Matti Hanni, and Perttu Lantto: *Supermolecular calculations of intermolecular interaction effects on NMR parameters. Examples on liquid water and gaseous xenon*, invited talk at the 13th European Seminar on Computational Methods in Quantum Chemistry, Smolenice, Slovak Republic, September 21–29, 2005 (Abstracts, L21).
4. **Juha Vaara**: *Relativistic computations of Xe NMR*, invited talk at the conference Relativistic effects in heavy-element chemistry and physics (REHE 2007), Domaine Saint-Jacques, Ottrott, France, March 21–25, 2007 (Abstracts, IL6).
5. **Juha Vaara**: *Computational xenon NMR*, invited talk at the 4th International Symposium on Xenon NMR of Materials (XeMat 2009), Ruka, Finland, June 7–10, 2009 (Proceedings, O8).
6. **Juha Vaara**: *Computational studies of anisotropic NMR observables*, invited talk at the conference NMR in oriented phases (Tropea 2009), Tropea, Italy, October 1–5, 2009.
7. **Juha Vaara**: *Calculations of nuclear spin optical rotation*, invited talk at EuroMagNET II Quantum chemistry in strong magnetic fields (QCSMF) workshop, Toulouse, France, September 13–14, 2010.
8. **Juha Vaara**: *Relativistic calculations of nuclear spin optical rotation and chemical shift anisotropy relaxation*, invited talk at the conference Relativistic effects in heavy-element chemistry and physics (REHE 2010), Beijing, China, September 25–29, 2010 (Abstracts, IL–22).
9. **Juha Vaara**: *Chemical distinction by nuclear spin optical rotation*, invited talk at the 52nd Experimental Nuclear Magnetic Resonance Conference (52nd ENC), Pacific Grove, USA, April 10–15, 2011 (Abstracts, p. 43).

Other

10. **Juha Vaara**, Olga L. Malkina, Bernd Schimmelpfennig, Hermann Stoll, Marketá Munzarová, Vladimir G. Malkin, and Martin Kaupp: *Density-functional calculations of spin-orbit effects in nuclear shielding and electronic g-tensors*, talk presented at Quantum Systems in Chemistry and Physics V (QSCP-V), Uppsala, Sweden, April 13–18, 2000.
11. **Juha Vaara** and Pekka Pyykkö: *Magnetic field-induced quadrupole splitting in gaseous ^{131}Xe : Quadratic and quartic field dependence*, talk presented at Hans Ågren Symposium in the Stockholm Environment 2000 (HASSE 2000), Villa Söderås, Lidingö, Sweden, September 30–October 1, 2000; talk presented at the 2001 Nordic NMR Symposium, Helsinki, August 26–29, 2001.
12. **Juha Vaara**: *Intermolecular effects on Xe chemical shifts*, talk presented at the final meeting of the EU/FP6 programme Understanding nanomaterials from the quantum perspective (NANOQUANT), Warsaw, Poland, March 17, 2007.
13. **Juha Vaara**, Teemu O. Pennanen, and Helmi Liimatainen: *Theory of nuclear magnetic resonance chemical shift in arbitrary electronic spin state*, talk presented at the 8th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC2008), Sydney, Australia, September 14–19, 2008.
14. **Juha Vaara**: *Molecular magnetism group*, talk presented at the Symposium on Modern Methods of Quantum Chemistry, Mariapfarr, Austria, March 4–8, 2009.

5. Talks at national conferences

1. **Juha Vaara**, Tapio T. Rantala, and Jukka Jokisaari: ^{21}Ne , ^{83}Kr and ^{131}Xe NMR: *A comparison of experiments with ab initio estimated relaxation rates*, talk presented at the XVI National NMR Symposium, Turku, Finland, June 3–4, 1993. Program and Abstracts, Meddelanden i serie B No. 130, Department of Organic Chemistry, Åbo Akademi University, Turku 1993.
2. **Juha Vaara**, Tapio T. Rantala, Juhani Lounila, Juha-Heikki Kantola and Jukka Jokisaari: *First principles computation of NMR parameters*, talk presented at the XVIII National NMR Symposium, Ikaalinen, Finland, June

12–14, 1996. Proceedings, Defence Forces Research Centre Publications A **10**, Ylöjärvi, 1996, p. 73–77.

3. **J. Vaara**, K. Ruud, O. Vahtras, H. Ågren, and J. Jokisaari: *Electronic spin-orbit interaction and NMR spectral parameters*, talk presented at The XXXII Annual Conference of the Finnish Physical Society, Tampere, Finland, March 19–21, 1998. Proceedings, Report 1-1998, Tampere University of Technology, Tampere 1998, 2.4.
4. **J. Vaara** and P. Pyykkö: *Magnetic field-induced quadrupole splitting in gaseous and liquid ^{131}Xe NMR: Quadratic and quartic field dependence*, talk presented at the XXXV Annual Conference of the Finnish Physical Society, Jyväskylä, Finland, March 22–24, 2001. Proceedings, Research Report No. 5/2001, Department of Physics, University of Jyväskylä, Jyväskylä, 2001, 8.1.
5. **Juha Vaara** and Pekka Pyykkö: *Dirac-Fock calculations of the nuclear magnetic shielding constants of noble gas atoms*, talk presented at the XXXVI Annual Conference of the Finnish Physical Society, Joensuu, Finland, March 14–16, 2002. Proceedings, Selected Papers 7, Department of Physics, University of Joensuu, Joensuu, 2002, 8.2.
6. **J. Vaara**, Z. Rinkevicius, L. Telyatnyk, and O. Vahtras: *Non-relativistic calculations of nuclear magnetic shielding in paramagnetic molecules*, talk presented at 25th Finnish NMR Symposium, Helsinki, Finland, June 5–7, 2003. Abstracts p. 19.
7. **Juha Vaara**: *NMR parameters from quantum-chemical computation*, talk presented at the XXVII Finnish NMR Symposium, Pudasjärvi, Finland, June 8–10, 2005. Abstracts L21.
8. **Juha Vaara**, Matti Hanni, Perttu Lantto, and Michal Straka: *Computational Xenon NMR*, talk presented at the XXIX Finnish NMR Symposium, Rymättylä, Finland, June 13–15, 2007. Abstracts, p. 30.

6. Other seminars and lectures

1. **Juha Vaara**: *First principles calculation of NMR parameters*, plenary lecture at the meeting "35 Years of NMR spectroscopy at the University of Oulu", University of Oulu, Oulu, Finland, September 18, 1997.

2. **Juha Vaara:** *Computational studies on the NMR parameters of molecular probes in liquids and solids*, lecture in the seminar series "Theory and computation of NMR and ESR parameters", Linköping University, Linköping, Sweden, December 1, 1997.
3. **Juha Vaara:** *Spin-orbit contributions to NMR spectral parameters*, lecture in the seminar series "Theory and computation of NMR and ESR parameters", Linköping University, Linköping, Sweden, December 1, 1997.
4. **Juha Vaara:** *NMR parameters - comparison between experiment and first principles theory*, seminar lecture, Institute of Organic Chemistry, Polish Academy Sciences, Warsaw, Poland, January 28, 1998.
5. **Juha Vaara:** *Ab initio calculations of the spin-orbit coupling contributions to NMR shielding and spin-spin coupling tensors*, seminar lecture, Graduiertenkolleg Magnetische Resonanz, Universität Stuttgart, Stuttgart, Germany, February 8, 1999.
6. **Juha Vaara:** *Density-functional calculation of relativistic corrections to parameters of magnetic resonance spectroscopy*, talk presented at the 3rd Marie Curie Fellows' Workshop, Max-Planck-Institut für Physik, Munich, Germany, October 25–27, 1999.
7. **Juha Vaara:** 1. *Kvanttikemian tutkimuksesta HY:n Kemian laitoksen Ruotsinkielisessä opetuslaboratoriossa*; 2. *Magneettisten resonanssispektroskopioiden (NMR ja ESR) parametrien teoria ja laskenta* (in Finnish), talk presented at the meeting of the CSC Physicists' network, CSC Scientific Computing Ltd., Espoo, December 19, 2001. *Theory and calculation of NMR and ESR parameters*, talk presented at the Soft Matter seminar series, Laboratory of Computational Engineering, Helsinki University of Technology, March 27, 2002, and in the seminar series of the Laboratory of Physical Chemistry, University of Helsinki, May 20, 2003.
8. **Juha Vaara:** *Theory and computation of magnetic resonance parameters*, talk presented at the Department of Physics, Tampere University of Technology, April 20, 2006.
9. **Juha Vaara:** *Theory of nuclear magneto-optic spectroscopy*, talk presented at the Department of Physics, Tampere University of Technology, November 26, 2010; talk presented at the Department of Chemistry and Materials Science, Aalto University, May 16, 2011.

10. **Juha Vaara:** *Molekyylimagnetismin teoria ja laskenta* (in Finnish), talk presented at the *CSC 40 years* seminar series, University of Oulu, March 25, 2011.

7. Other publications

1. **Juha Vaara:** *Two-point magnetoconductance and intermode scattering in ballistic constrictions*, Diploma thesis, University of Oulu, Department of Electrical Engineering, 1992.
2. **Juha Vaara**, Tapio T. Rantala, Juhani Lounila, Juha-Heikki Kantola, and Jukka Jokisaari: *Computational studies of NMR parameters of molecular probes in liquids and solids*, *CSC News* **8**, 7–9 (1996).
3. **Juha Vaara:** *Computational studies on the NMR parameters of molecular probes in liquids and solids*, Report Series in Physical Sciences No 7, University of Oulu, Department of Physical Sciences, 1997 (Ph.D. thesis).
4. **Juha Vaara:** *Theory and calculations of NMR and EPR parameters*, CSC Report on Scientific Computing 1999–2000, S. Kotila and J. Haataja, eds. (CSC - Scientific Computing Ltd, 2001), pp. 118–121.
5. H. Korschin, N. Runeberg, D. Sundholm, and **J. Vaara:** *Tarkkoja työkaluja monitieteelliseen tutkimukseen. Kansainvälinen kvanttikemian konferenssi Kuusamossa* (in Finnish), *Kemia-Kemi* **29**, 52 (2002).
6. **Juha Vaara:** *Theory and quantum-chemical calculation of magnetic resonance parameters*, CSC Report on Scientific Computing in Finland 2004–2005, J. Fagerholm, L. Puska, J. Åström, J. Blomqvist, P.-L. Forsström, L. Jukka, S. Kotila, M. M. Laine, M. Miettinen, J. Tarus, and S. Tissari, eds. (CSC -Scientific Computing Ltd, 2005), pp. 106–109.
7. **Juha Vaara:** *Laskennallinen magneettisen resonanssin tutkimus: Silta spektrien ja molekyyli mallien välillä* (in Finnish), *Tietoyhteys* 2/2006, pp. 10–12.

Oulu, August 5, 2011,

Juha Vaara