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Publications and Conference Papers

2014

1. Ville J. Härkönen and Antti J. Karttunen, ***Ab initio* lattice dynamical studies of silicon clathrate frameworks and their negative thermal expansion**, Physical Review B, DOI: 10.1103/PhysRevB.89.024305
2. L.-j. Fu and J. Vaara, **Nuclear quadrupole moment-induced Cotton-Mouton effect in molecules**, Journal of Chemical Physics 140, 024103, DOI: 10.1063/1.4855315 >>

2013

1. N. Abuzaid, A. M. Kantola, and J. Vaara, **Magnetic field-induced nuclear quadrupole coupling in atomic ¹³¹Xe**, Molecular Physics 111, 1390-1400, DOI: 10.1080/00268976.2013.793840 >>
2. L.-j. Fu and J. Vaara, **Nuclear spin-induced Cotton-Mouton effect in molecules**, Journal of Chemical Physics 138, 204110, DOI: 10.1063/1.4807396 >>
3. L.-j. Fu, A. Rizzo and J. Vaara, **Nuclear quadrupole moment-induced Cotton-Mouton effect in noble gas atoms**, Journal of Chemical Physics 139, 181102:1-4, DOI: 10.1063/1.4830094 >>
4. J. Jokisaari and J. Vaara, **Nuclear spin-spin coupling anisotropy in van der Waals-bonded ¹²⁹Xe dimer**, Physical Chemistry Chemical Physics 15, 11427-11430, DOI: 10.1039/c3cp50625h >>
5. J. Karjalainen, J. Lintuvuori, V.-V. Telkki, P. Lantto, and J. Vaara, **Constant-pressure simulations of Gay-Berne liquid-crystalline phases in cylindrical nanocavities**, Physical Chemistry Chemical Physics, 15, 14047-14057, DOI: 10.1039/C3CP51241J >>
6. P. Lantto, S. Kangasvieri, and J. Vaara, **Electron correlation and relativistic effects in the secondary NMR isotope shifts of CSe₂**, Physical Chemistry Chemical Physics, 15, 17468-17478, DOI: 10.1039/C3CP51904J >>
7. J. Precechtelova, M. L. Munzarova, J. Vaara, J. Novotny, M. Dracinsky, and V. Sklenar, **Towards Reproducing Sequence Trends in Phosphorus Chemical Shifts for Nucleic Acids by MD/DFT Calculations**, Journal of Chemical Theory and Computation 9, 1641-1656, DOI: 10.1021/ct300488y >>
8. J. Shi, S. Ikäläinen, J. Vaara, and M. V. Romalis, **Observation of optical chemical shift by precision nuclear spin optical rotation measurements and calculations**, Journal of Physical Chemistry Letters 4, 437-441, DOI: 10.1021/jz3018539 >>
9. J. Vaara, M. Hanni and J. Jokisaari, **Nuclear spin-spin coupling in a van der Waals-bonded system: Xenon dimer**, Journal of Chemical Physics 138, 104313, DOI: 10.1063/1.4793745 >>
10. J. Vähäkangas, S. Ikäläinen, P. Lantto, and J. Vaara, **Nuclear Magnetic Resonance Predictions for Graphenes: Concentric Finite Models and Extrapolation to Large Systems**, Physical Chemistry Chemical Physics 15, 4634-4641, DOI: 10.1039/c3cp44631j >>
11. J. Vaara, **Chemical Shift in Paramagnetic Systems**, in High Resolution NMR Spectroscopy Vol. 3, pp. 41-67, ed R. H. Contreras, Elsevier: Amsterdam, DOI: 10.1016/B978-0-444-59411-2.00003-4 >>

2012

1. S. Ikäläinen, P. Lantto, and J. Vaara, **Fully relativistic calculations of Faraday and nuclear spin-induced optical rotation in xenon**, Journal of Chemical Theory and Computation, 8, 91-98, DOI: 10.1021/ct200636m >>
2. P. Lantto, S. Standara, S. Riedel, J. Vaara, and M. Straka, **Exploring New ¹²⁹Xe Chemical Shift Ranges in HXeY Compounds: Hydrogen More Relativistic than Xenon**, Physical Chemistry Chemical Physics, 14, 10944-10952, DOI: 10.1039/C2CP41240C >>
3. P. Lantto, S. Kangasvieri, J. Vaara, **Rovibrational effects on NMR shieldings in a heavy-element system: XeF₂**, Journal of Chemical Physics, 137, 214309:1-10, DOI: 10.1063/1.4768471 >>
4. T. S. Pennanen, S. Ikäläinen, P. Lantto, and J. Vaara, **Nuclear spin optical rotation and Faraday effect in gaseous and liquid water**, Journal of Chemical Physics, 136, 184502:1-6, DOI: 10.1063/1.4711957 >>