

# CSEC Publications 2014

## Record 1 of 57

**Title:** Synthesis, anion order and magnetic properties of RVO<sub>3</sub>-xN<sub>x</sub> perovskites (R = La, Pr, Nd; 0 ≤ x ≤ 1)

**Author(s):** Oro-Sole, J (Oro-Sole, Judith); Clark, L (Clark, Lucy); Kumar, N (Kumar, Nitesh); Bonin, W (Bonin, William); Sundaresan, A (Sundaresan, A.); Attfield, JP (Attfield, J. Paul); Rao, CNR (Rao, C. N. R.); Fuertes, A (Fuertes, Amparo)

**Source:** JOURNAL OF MATERIALS CHEMISTRY C **Volume:** 2 **Issue:** 12 **Pages:** 2212-2220 **DOI:** 10.1039/c3tc32362e **Published:** 2014

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## Record 2 of 57

**Title:** Enteric YaiW Is a Surface-Exposed Outer Membrane Lipoprotein That Affects Sensitivity to an Antimicrobial Peptide

**Author(s):** Arnold, MFF (Arnold, Markus F. F.); Caro-Hernandez, P (Caro-Hernandez, Paola); Tan, K (Tan, Karen); Runti, G (Runti, Giulia); Wehmeier, S (Wehmeier, Silvia); Scocchi, M (Scocchi, Marco); Doerfler, WT (Doerfler, William T.); Walker, GC (Walker, Graham C.); Ferguson, GP (Ferguson, Gail P.)

**Source:** JOURNAL OF BACTERIOLOGY **Volume:** 196 **Issue:** 2 **Pages:** 436-444 **DOI:** 10.1128/JB.01179-13 **Published:** JAN 2014

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## Record 3 of 57

**Title:** The effect of pressure on the post-synthetic modification of a nanoporous metal-organic framework

**Author(s):** McKellar, SC (McKellar, Scott C.); Graham, AJ (Graham, Alexander J.); Allan, DR (Allan, David R.); Mohideen, MIH (Mohideen, M. Infas H.); Morris, RE (Morris, Russell E.); Moggach, SA (Moggach, Stephen A.)

**Source:** NANOSCALE **Volume:** 6 **Issue:** 8 **Pages:** 4163-4173 **DOI:** 10.1039/c3nr04161a **Published:** 2014

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## Record 4 of 57

**Title:** High pressure neutron and X-ray diffraction at low temperatures

**Author(s):** Ridley, CJ (Ridley, Christopher J.); Kamenev, KV (Kamenev, Konstantin V.)

**Source:** ZEITSCHRIFT FUR KRISTALLOGRAPHIE **Volume:** 229 **Issue:** 3 **Special Issue:** SI **Pages:** 171-199 **DOI:** 10.1515/zkri-2013-1673 **Part:** 2 **Published:** 2014

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## Record 5 of 57

**Title:** A pressure-induced displacive phase transition in Tris(ethylenediamine) Nickel(II) nitrate

**Author(s):** Cameron, CA (Cameron, Christopher A.); Allan, DR (Allan, David R.); Kamenev, KV (Kamenev, Konstantin V.); Moggach, SA (Moggach, Stephen A.); Murrice, M (Murrice, Mark); Parsons, S (Parsons, Simon)

**Source:** ZEITSCHRIFT FUR KRISTALLOGRAPHIE **Volume:** 229 **Issue:** 3 **Special Issue:** SI **Pages:** 200-209 **DOI:** 10.1515/zkri-2013-1688 **Part:** 2 **Published:** 2014

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## Record 6 of 57

**Title:** Structural characterization of sodium azide and sodium bifluoride at high pressures

**Author(s):** Millar, DIA (Millar, David I. A.); Barry, C (Barry, Christopher); Marshall, WG (Marshall, William G.); Pulham, CR (Pulham, Colin R.)

**Source:** ZEITSCHRIFT FUR KRISTALLOGRAPHIE **Volume:** 229 **Issue:** 3 **Special Issue:** SI **Pages:** 259-275 **DOI:** 10.1515/zkri-2013-1660 **Part:** 2 **Published:** 2014

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## Record 7 of 57

**Title:** Competition between hydrogen bonding and dispersion interactions in the crystal structures of the primary amines

**Author(s):** Maloney, AGP (Maloney, Andrew G. P.); Wood, PA (Wood, Peter A.); Parsons, S (Parsons, Simon)

**Source:** CRYSTENGCOMM **Volume:** 16 **Issue:** 19 **Pages:** 3867-3882 **DOI:** 10.1039/c3ce42639d **Published:** 2014

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## Record 8 of 57

**Title:** High pressure polymorphism of beta-TaON

**Author(s):** Woodhead, K (Woodhead, K.); Pascarelli, S (Pascarelli, S.); Hector, AL (Hector, A. L.); Briggs, R (Briggs, R.); Alderman, N (Alderman, N.); McMillan, PF (McMillan, P. F.)

**Source:** DALTON TRANSACTIONS **Volume:** 43 **Issue:** 25 **Pages:** 9647-9654 **DOI:** 10.1039/c4dt00805g **Published:** 2014

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## Record 9 of 57

**Title:** High temperature Raman analysis of hydrogen phase IV from molecular dynamics

**Author(s):** Magdau, IB (Magdau, I. B.); Ackland, GJ (Ackland, G. J.)

**Edited by:** Buttler W; Furlanetto M; Evans W

**Source:** 18TH APS-SCCM AND 24TH AIRAPT, PTS 1-19 **Book Series:** Journal of Physics Conference Series **Volume:** 500 **Article Number:** 032012 **DOI:** 10.1088/1742-6596/500/3/032012 **Published:** 2014

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## Record 10 of 57

**Title:** Re-entrant layer reconstruction during intercalation in hafnium nitride chloride

**Author(s):** Meignen, V (Meignen, Vincent); Oro-Sole, J (Oro-Sole, Judith); Bonin, W (Bonin, William); Morcrette, M (Morcrette, Mathieu); Palacin, MR (Palacin, M. Rosa); Attfield, JP (Attfield, J. Paul); Fuertes, A (Fuertes, Amparo)

**Source:** CHEMICAL SCIENCE **Volume:** 5 **Issue:** 8 **Pages:** 2974-2978 **DOI:** 10.1039/c4sc00499j **Published:** 2014

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## Record 11 of 57

**Title:** Comparison of intermolecular interactions in two phases of MeNSOF<sub>2</sub>

**Author(s):** Mews, R (Mews, Ruediger); Parsons, S (Parsons, Simon)

**Source:** ZEITSCHRIFT FUR KRISTALLOGRAPHIE **Volume:** 229 **Issue:** 9 **Special Issue:** SI **Pages:** 649-660 **DOI:** 10.1515/zkri-2014-1733 **Published:** 2014

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## Record 12 of 57

**Title:** A high-pressure polymorph of propionamide from in situ high-pressure crystallisation from solution

**Author(s):** Fabbiani, FPA (Fabbiani, Francesca P. A.); Pulham, CR (Pulham, Colin R.); Warren, JE (Warren, John E.)

**Source:** ZEITSCHRIFT FUR KRISTALLOGRAPHIE **Volume:** 229 **Issue:** 9 **Special Issue:** SI **Pages:** 667-675 **DOI:** 10.1515/zkri-2014-1728 **Published:** 2014

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## Record 13 of 57

**Title:** Effect of high pressure on the crystal structure and charge transport properties of the (2-fluoro-3-pyridyl)(4-iodophenyl)boronic 8-oxyquinolate complex

**Author(s):** Wesela-Bauman, G (Wesela-Bauman, Grzegorz); Parsons, S (Parsons, Simon); Serwatowski, J (Serwatowski, Janusz); Wozniak, K (Wozniak, Krzysztof)

**Source:** CRYSTENGCOMM **Volume:** 16 **Issue:** 47 **Pages:** 10780-10790 **DOI:** 10.1039/c4ce01730g **Published:** 2014

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## Record 14 of 57

**Title:** Magnetic excitations in the ferromagnetic superconductor UGe<sub>2</sub> under pressure.

**Author(s):** Kapa, MW (Kapa, M. W.); Sokolov, DA (Sokolov, D. A.); Bohm, M (Bohm, M.); Huxley, AD (Huxley, A. D.)

**Edited by:** Calzetta E

**Source:** 27TH INTERNATIONAL CONFERENCE ON LOW TEMPERATURE PHYSICS (LT27), PTS 1-5 **Book Series:** Journal of Physics Conference Series **Volume:** 568 **Article Number:** 042016 **DOI:** 10.1088/1742-6596/568/4/042016 **Published:** 2014

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## Record 15 of 57

**Title:** Wigner-Mott insulator-to-insulator transition at pressure in charge-ordered Fe<sub>2</sub>OBO<sub>3</sub>

**Author(s):** Diguët, G (Diguët, G.); Hearne, GR (Hearne, G. R.); Sibanda, WN (Sibanda, W. N.); Carleschi, E (Carleschi, E.); Musyimi, P (Musyimi, P.); Pischedda, V (Pischedda, V.); Attfield, JP (Attfield, J. P.)

**Source:** PHYSICAL REVIEW B **Volume:** 89 **Issue:** 3 **Article Number:** 035132 **DOI:** 10.1103/PhysRevB.89.035132 **Published:** JAN 21 2014

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## Record 16 of 57

**Title:** Magnetic properties of nano-scale hematite, alpha-Fe<sub>2</sub>O<sub>3</sub>, studied by time-of-flight inelastic neutron spectroscopy

**Author(s):** Hill, AH (Hill, Adrian H.); Jacobsen, H (Jacobsen, Henrik); Stewart, JR (Stewart, J. Ross); Jiao, F (Jiao, Feng); Jensen, NP (Jensen, Niels P.); Holm, SL (Holm, Sonja L.); Mutka, H (Mutka, Hannu); Seydel, T (Seydel, Tilo); Harrison, A (Harrison, Andrew); Lefmann, K (Lefmann, Kim)

**Source:** JOURNAL OF CHEMICAL PHYSICS **Volume:** 140 **Issue:** 4 **Article Number:** 044709 **DOI:** 10.1063/1.4862235 **Published:** JAN 28 2014

**Record 17 of 57**

**Title:** Mechanism for radiation damage resistance in yttrium oxide dispersion strengthened steels

**Author(s):** Brodrick, J (Brodrick, J.); Hepburn, DJ (Hepburn, D. J.); Ackland, GJ (Ackland, G. J.)

**Source:** JOURNAL OF NUCLEAR MATERIALS **Volume:** 445 **Issue:** 1-3 **Pages:** 291-297 **DOI:** 10.1016/j.jnucmat.2013.10.045 **Published:** FEB 2014

**Record 18 of 57**

**Title:** Control of L-type Ferrimagnetism by the Ce/Vacancy Ordering in the A-Site-Ordered Perovskite Ce<sub>1/2</sub>Cu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub>

**Author(s):** Saito, T (Saito, Takashi); Yamada, R (Yamada, Ryuta); Ritter, C (Ritter, Clemens); Senn, MS (Senn, Mark S.); Atfield, JP (Atfield, J. Paul); Shimakawa, Y (Shimakawa, Yuichi)

**Source:** INORGANIC CHEMISTRY **Volume:** 53 **Issue:** 3 **Pages:** 1578-1584 **DOI:** 10.1021/ic402616r **Published:** FEB 3 2014

**Record 19 of 57**

**Title:** Chemical pressure effects on magnetism in the quantum spin liquid candidates Yb<sub>2</sub>X<sub>2</sub>O<sub>7</sub> (X = Sn, Ti, Ge)

**Author(s):** Dun, ZL (Dun, Z. L.); Lee, M (Lee, M.); Choi, ES (Choi, E. S.); Hallas, AM (Hallas, A. M.); Wiebe, CR (Wiebe, C. R.); Gardner, JS (Gardner, J. S.); Arrighi, E (Arrighi, E.); Freitas, RS (Freitas, R. S.); Arevalo-Lopez, AM (Arevalo-Lopez, A. M.); Atfield, JP (Atfield, J. P.); Zhou, HD (Zhou, H. D.); Cheng, JG (Cheng, J. G.)

**Source:** PHYSICAL REVIEW B **Volume:** 89 **Issue:** 6 **Article Number:** 064401 **DOI:** 10.1103/PhysRevB.89.064401 **Published:** FEB 4 2014

**Record 20 of 57**

**Title:** Long-range antiferromagnetic order in the frustrated XY pyrochlore antiferromagnet Er<sub>2</sub>Ge<sub>2</sub>O<sub>7</sub>

**Author(s):** Li, X (Li, X.); Li, WM (Li, W. M.); Matsubayashi, K (Matsubayashi, K.); Sato, Y (Sato, Y.); Jin, CQ (Jin, C. Q.); Uwatoko, Y (Uwatoko, Y.); Kawae, T (Kawae, T.); Hallas, AM (Hallas, A. M.); Wiebe, CR (Wiebe, C. R.); Arevalo-Lopez, AM (Arevalo-Lopez, A. M.); Atfield, JP (Atfield, J. P.); Gardner, JS (Gardner, J. S.); Freitas, RS (Freitas, R. S.); Zhou, HD (Zhou, H. D.); Cheng, JG (Cheng, J. G.)

**Source:** PHYSICAL REVIEW B **Volume:** 89 **Issue:** 6 **Article Number:** 064409 **DOI:** 10.1103/PhysRevB.89.064409 **Published:** FEB 12 2014

**Record 21 of 57**

**Title:** Clumped fluoride-hydroxyl defects in forsterite: Implications for the upper-mantle

**Author(s):** Creppison, C (Creppison, Celine); Blanchard, M (Blanchard, Marc); Bureau, H (Bureau, Helene); Sanloup, C (Sanloup, Chryste); Withers, AC (Withers, Anthony C.); Khodja, H (Khodja, Hicham); Surble, S (Surble, Suzy); Raepsaet, C (Raepsaet, Caroline); Beneut, K (Beneut, Keevin); Leroy, C (Leroy, Clemence); Giura, P (Giura, Paola); Balan, E (Balan, Etienne)

**Source:** EARTH AND PLANETARY SCIENCE LETTERS **Volume:** 390 **Pages:** 287-295 **DOI:** 10.1016/j.epsl.2014.01.020 **Published:** MAR 15 2014

**Record 22 of 57**

**Title:** Solid solutions and phase transitions in (Ca,M<sub>2+</sub>)M<sub>2</sub>+Si<sub>2</sub>O<sub>6</sub> pyroxenes (M<sub>2+</sub> = Co, Fe, Mg)

**Author(s):** Mantovani, L (Mantovani, Luciana); Tribaudino, M (Tribaudino, Mario); Bertoni, G (Bertoni, Giovanni); Salviati, G (Salviati, Giancarlo); Bromiley, G (Bromiley, Geoffrey)

**Source:** AMERICAN MINERALOGIST **Volume:** 99 **Issue:** 4 **Pages:** 704-711 **DOI:** 10.2138/am.2014.4684 **Published:** APR 2014

**Record 23 of 57**

**Title:** High-pressure cell for neutron diffraction with in situ pressure control at cryogenic temperatures

**Author(s):** Jacobsen, MK (Jacobsen, Matthew K.); Ridley, CJ (Ridley, Christopher J.); Bocian, A (Bocian, Artur); Kirichek, O (Kirichek, Oleg); Manuel, P (Manuel, Pascal); Khalyavin, D (Khalyavin, Dmitry); Azuma, M (Azuma, Masaki); Atfield, JP (Atfield, J. Paul); Kamenev, KV (Kamenev, Konstantin V.)

**Source:** REVIEW OF SCIENTIFIC INSTRUMENTS **Volume:** 85 **Issue:** 4 **Article Number:** 043904 **DOI:** 10.1063/1.4870061 **Published:** APR 2014

**Record 24 of 57**

**Title:** Investigation of Acrylic Acid at High Pressure Using Neutron Diffraction

**Author(s):** Johnston, BF (Johnston, Blair F.); Marshall, WG (Marshall, William G.); Parsons, S (Parsons, Simon); Urquhart, AJ (Urquhart, Andrew J.); Oswald, IDH (Oswald, Iain D. H.)

**Source:** JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 118 **Issue:** 14 **Pages:** 4044-4051 **DOI:** 10.1021/jp502095n **Published:** APR 10 2014

**Record 25 of 57**

**Title:** Strong Increase of T<sub>c</sub> of Sr<sub>2</sub>RuO<sub>4</sub> Under Both Tensile and Compressive Strain

**Author(s):** Hicks, CW (Hicks, Clifford W.); Brodsky, DO (Brodsky, Daniel O.); Yelland, EA (Yelland, Edward A.); Gibbs, AS (Gibbs, Alexandra S.); Bruin, JAN (Bruin, Jan A. N.); Barber, ME (Barber, Mark E.); Edkins, SD (Edkins, Stephen D.); Nishimura, K (Nishimura, Keigo); Yonezawa, S (Yonezawa, Shingo); Maeno, Y (Maeno, Yoshiteru); Mackenzie, AP (Mackenzie, Andrew P.)

**Source:** SCIENCE **Volume:** 344 **Issue:** 6181 **Pages:** 283-285 **DOI:** 10.1126/science.1248292 **Published:** APR 18 2014

**Record 26 of 57**

**Title:** Magmas trapped at the continental lithosphere-asthenosphere boundary

**Author(s):** Creppison, C (Creppison, C.); Morard, G (Morard, G.); Bureau, H (Bureau, H.); Prouteau, G (Prouteau, G.); Morizet, Y (Morizet, Y.); Petitgirard, S (Petitgirard, S.); Sanloup, C (Sanloup, C.)

**Source:** EARTH AND PLANETARY SCIENCE LETTERS **Volume:** 393 **Pages:** 105-112 **DOI:** 10.1016/j.epsl.2014.02.048 **Published:** MAY 1 2014

**Record 27 of 57**

**Title:** High Pressure Synthesis of the Cation-ordered Perovskite 3C1: 2-Ba<sub>3</sub>NaRu<sub>2</sub>O<sub>9</sub>

**Author(s):** Arevalo-Lopez, AM (Arevalo-Lopez, Angel M.); Senn, MS (Senn, Mark S.); Skedd, L (Skedd, Lauren); Atfield, JP (Atfield, J. Paul)

**Source:** ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE **Volume:** 640 **Issue:** 6 **Special Issue:** SI **Pages:** 1164-1167 **DOI:** 10.1002/zaac.201300549 **Published:** MAY 2014

**Record 28 of 57**

**Title:** A half-metallic A- and B-site-ordered quadruple perovskite oxide CaCu<sub>3</sub>Fe<sub>2</sub>Re<sub>2</sub>O<sub>12</sub> with large magnetization and a high transition temperature

**Author(s):** Chen, WT (Chen, Wei-tin); Mizumaki, M (Mizumaki, Masaichiro); Seki, H (Seki, Hayato); Senn, MS (Senn, Mark S.); Saito, T (Saito, Takashi); Kan, D (Kan, Daisuke); Atfield, JP (Atfield, J. Paul); Shimakawa, Y (Shimakawa, Yuichi)

**Source:** NATURE COMMUNICATIONS **Volume:** 5 **Article Number:** 3909 **DOI:** 10.1038/ncomms4909 **Published:** MAY 2014

**Record 29 of 57**

**Title:** Evolution of the 4f electron localization from YbRh<sub>2</sub>Si<sub>2</sub> to YbRh<sub>2</sub>Pb studied by electron spin resonance

**Author(s):** Ivanshin, VA (Ivanshin, V. A.); Litvinova, TO (Litvinova, T. O.); Ivanshin, NA (Ivanshin, N. A.); Poppl, A (Poepl, A.); Sokolov, DA (Sokolov, D. A.); Aronson, MC (Aronson, M. C.)

**Source:** JOURNAL OF EXPERIMENTAL AND THEORETICAL PHYSICS **Volume:** 118 **Issue:** 5 **Pages:** 760-764 **DOI:** 10.1134/S1063776114050033 **Published:** MAY 2014

**Record 30 of 57**

**Title:** An improved method for calibrating time-of-flight Laue single-crystal neutron diffractometers

**Author(s):** Bull, CL (Bull, Craig L.); Johnson, MW (Johnson, Michael W.); Hamidov, H (Hamidov, Hayrullo); Komatsu, K (Komatsu, Kazuki); Guthrie, M (Guthrie, Malcolm); Gutmann, MJ (Gutmann, Matthias J.); Loveday, JS (Loveday, John S.); Nelmes, RJ (Nelms, Richard J.)

**Source:** JOURNAL OF APPLIED CRYSTALLOGRAPHY **Volume:** 47 **Pages:** 974-983 **DOI:** 10.1107/S1600576714006657 **Part:** 3 **Published:** JUN 2014

**Record 31 of 57**

**Title:** Efficacious calculation of Raman spectra in high pressure hydrogen

**Author(s):** Ackland, GJ (Ackland, G. J.); Magdau, IB (Magdau, I. B.)

**Source:** HIGH PRESSURE RESEARCH **Volume:** 34 **Issue:** 2 **Pages:** 198-204 **DOI:** 10.1080/08957959.2013.856897 **Published:** JUN 2014

**Record 32 of 57**

**Title:** Stabilization of Scandium Terephthalate MOFs against Reversible Amorphization and Structural Phase Transition by Guest Uptake at Extreme Pressure

**Author(s):** Graham, AJ (Graham, Alexander J.); Banu, AM (Banu, Ana-Maria); Duren, T (Dueren, Tina); Greenaway, A (Greenaway, Alex); McKellar, SC (McKellar, Scott C.); Mowat, JPS (Mowat, John P. S.); Ward, K (Ward, Kenneth); Wright, PA (Wright, Paul A.); Moggach, SA (Moggach, Stephen A.)

**Source:** JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 136 **Issue:** 24 **Pages:** 8606-8613 **DOI:** 10.1021/ja411934f **Published:** JUN 18 2014

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**Record 33 of 57**

**Title:** Lithium hydroxide, LiOH, at elevated densities

**Author(s):** Hermann, A (Hermann, Andreas); Ashcroft, NW (Ashcroft, N. W.); Hoffmann, R (Hoffmann, Roald)

**Source:** JOURNAL OF CHEMICAL PHYSICS **Volume:** 141 **Issue:** 2 **Article Number:** 024505 **DOI:** 10.1063/1.4886335 **Published:** JUL 2014

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**Record 34 of 57**

**Title:** Spin-Wave Spectrum of the Quantum Ferromagnet on the Pyrochlore Lattice Lu<sub>2</sub>V<sub>2</sub>O<sub>7</sub>

**Author(s):** Mena, M (Mena, M.); Perry, RS (Perry, R. S.); Perring, TG (Perring, T. G.); Le, MD (Le, M. D.); Guerrero, S (Guerrero, S.); Storni, M (Storni, M.); Adroja, DT (Adroja, D. T.); Ruegg, C (Ruegg, Ch.); McMorrow, DF (McMorrow, D. F.)

**Source:** PHYSICAL REVIEW LETTERS **Volume:** 113 **Issue:** 4 **Article Number:** 047202 **DOI:** 10.1103/PhysRevLett.113.047202 **Published:** JUL 23 2014

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**Record 35 of 57**

**Title:** High-pressure effect on the superconductivity of YB<sub>6</sub>

**Author(s):** Gabani, S (Gabani, S.); Takacova, I (Takacova, I.); Pristas, G (Pristas, G.); Gazo, E (Gazo, E.); Flachbart, K (Flachbart, K.); Mori, T (Mori, T.); Braithwaite, D (Braithwaite, D.); Misek, M (Misek, M.); Kamenev, KV (Kamenev, K. V.); Hanfland, M (Hanfland, M.); Samuely, P (Samuely, P.)

**Source:** PHYSICAL REVIEW B **Volume:** 90 **Issue:** 4 **DOI:** 10.1103/PhysRevB.90.045136 **Published:** JUL 28 2014

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**Record 36 of 57**

**Title:** Review of modern instrumentation for magnetic measurements at high pressure and low temperature

**Author(s):** Wang, X (Wang, X.); Kamenev, KV (Kamenev, K. V.)

**Source:** LOW TEMPERATURE PHYSICS **Volume:** 40 **Issue:** 8 **Pages:** 735-746 **DOI:** 10.1063/1.4892645 **Published:** AUG 2014

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**Record 37 of 57**

**Title:** Synthesis and Properties of Lanthanide Ruthenium(III) Oxide Perovskites

**Author(s):** Sinclair, A (Sinclair, Alexandra); Rodgers, JA (Rodgers, Jennifer A.); Topping, CV (Topping, Craig V.); Misek, M (Misek, Martin); Stewart, RD (Stewart, Ross D.); Kockelmann, W (Kockelmann, Winfried); Bos, JWG (Bos, Jan-Willem G.); Atfield, JP (Atfield, J. Paul)

**Source:** ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 53 **Issue:** 32 **Pages:** 8343-8347 **DOI:** 10.1002/anie.201403223 **Published:** AUG 4 2014

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**Record 38 of 57**

**Title:** B-Cation Order Control of Magnetism in the 1322 Perovskite CaCu<sub>3</sub>Fe<sub>2</sub>Nb<sub>2</sub>O<sub>12</sub>

**Author(s):** Senn, MS (Senn, Mark S.); Chen, WT (Chen, Wei-tin); Saito, T (Saito, Takashi); Garcia-Martin, S (Garcia-Martin, Susana); Atfield, JP (Atfield, J. Paul); Shimakawa, Y (Shimakawa, Yuichi)

**Source:** CHEMISTRY OF MATERIALS **Volume:** 26 **Issue:** 16 **Pages:** 4832-4837 **DOI:** 10.1021/cm502064b **Published:** AUG 26 2014

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**Record 39 of 57**

**Title:** High-pressure X-ray science on the ultimate storage ring

**Author(s):** McMahan, MI (McMahon, Malcolm I.)

**Source:** JOURNAL OF SYNCHROTRON RADIATION **Volume:** 21 **Pages:** 1077-1083 **DOI:** 10.1107/S1600577514012855 **Part:** 5 **Published:** SEP 2014

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**Record 40 of 57**

**Title:** From Spin Glass to Quantum Spin Liquid Ground States in Molybdate Pyrochlores

**Author(s):** Clark, L (Clark, L.); Nilsen, GJ (Nilsen, G. J.); Kermarrec, E (Kermarrec, E.); Ehlers, G (Ehlers, G.); Knight, KS (Knight, K. S.); Harrison, A (Harrison, A.); Atfield, JP (Atfield, J. P.); Gaulin, BD (Gaulin, B. D.)

**Source:** PHYSICAL REVIEW LETTERS **Volume:** 113 **Issue:** 11 **Article Number:** 117201 **DOI:** 10.1103/PhysRevLett.113.117201 **Published:** SEP 8 2014

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**Record 41 of 57**

**Title:** High-Pressure Transformation of SiO<sub>2</sub> Glass from a Tetrahedral to an Octahedral Network: A Joint Approach Using Neutron Diffraction and Molecular Dynamics

**Author(s):** Zeidler, A (Zeidler, Anita); Wezka, K (Wezka, Kamil); Rowlands, RF (Rowlands, Ruth F.); Whittaker, DAJ (Whittaker, Dean A. J.); Salmon, PS (Salmon, Philip S.); Polidori, A (Polidori, Annalisa); Drewitt, JWE (Drewitt, James W. E.); Klotz, S (Klotz, Stefan); Fischer, HE (Fischer, Henry E.); Wilding, MC (Wilding, Martin C.); Bull, CL (Bull, Craig L.); Tucker, MG (Tucker, Matthew G.); Wilson, M (Wilson, Mark)

**Source:** PHYSICAL REVIEW LETTERS **Volume:** 113 **Issue:** 13 **Article Number:** 135501 **DOI:** 10.1103/PhysRevLett.113.135501 **Published:** SEP 23 2014

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**Record 42 of 57**

**Title:** In situ synchrotron X-ray diffraction in the laser-heated diamond anvil cell: Melting phenomena and synthesis of new materials

**Author(s):** Salamat, A (Salamat, Ashkan); Fischer, RA (Fischer, Rebecca A.); Briggs, R (Briggs, Richard); McMahan, MI (McMahon, Malcolm I.); Petitgirard, S (Petitgirard, Sylvain)

**Source:** COORDINATION CHEMISTRY REVIEWS **Volume:** 277 **Special Issue:** SI **Pages:** 15-30 **DOI:** 10.1016/j.ccr.2014.01.034 **Published:** OCT 1 2014

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**Record 43 of 57**

**Title:** CH<sub>3</sub>N=SF<sub>2</sub>=NCH<sub>3</sub>: Structural, Conformational, and Configurational Properties in the Gaseous and in the Condensed Phases

**Author(s):** Robles, NL (Robles, Norma L.); Parsons, S (Parsons, Simon); Mews, R (Mews, Ruediger); Oberhammer, H (Oberhammer, Heinz)

**Source:** EUROPEAN JOURNAL OF INORGANIC CHEMISTRY **Issue:** 30 **Pages:** 5185-5192 **DOI:** 10.1002/ejic.201402523 **Published:** OCT 2014

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**Record 44 of 57**

**Title:** Use of an advanced composite material in construction of a high pressure cell for magnetic ac susceptibility measurements

**Author(s):** Wang, X (Wang, X.); Misek, M (Misek, M.); Jacobsen, MK (Jacobsen, M. K.); Kamenev, KV (Kamenev, K. V.)

**Source:** HIGH PRESSURE RESEARCH **Volume:** 34 **Issue:** 4 **Pages:** 371-384 **DOI:** 10.1080/08957959.2014.977276 **Published:** OCT 2 2014

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**Record 45 of 57**

**Title:** Liquid iron-sulfur alloys at outer core conditions by first-principles calculations

**Author(s):** Umemoto, K (Umemoto, Koichiro); Hirose, K (Hirose, Kei); Imada, S (Imada, Saori); Nakajima, Y (Nakajima, Yoichi); Komabayashi, T (Komabayashi, Tetsuya); Tsutsui, S (Tsutsui, Satoshi); Baron, AQR (Baron, Alfred Q. R.)

**Source:** GEOPHYSICAL RESEARCH LETTERS **Volume:** 41 **Issue:** 19 **Pages:** 6712-6717 **DOI:** 10.1002/2014GL061233 **Published:** OCT 16 2014

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**Record 46 of 57**

**Title:** Equation of state and high-pressure/high-temperature phase diagram of magnesium

**Author(s):** Stinton, GW (Stinton, G. W.); MacLeod, SG (MacLeod, S. G.); Cynn, H (Cynn, H.); Errandonea, D (Errandonea, D.); Evans, WJ (Evans, W. J.); Proctor, JE (Proctor, J. E.); Meng, Y (Meng, Y.); McMahan, MI (McMahon, M. I.)

**Source:** PHYSICAL REVIEW B **Volume:** 90 **Issue:** 13 **Article Number:** 134105 **DOI:** 10.1103/PhysRevB.90.134105 **Published:** OCT 20 2014

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**Record 47 of 57**

**Title:** Phonon Localization by Mass Disorder in Dense Hydrogen-Deuterium Binary Alloy

**Author(s):** Howie, RT (Howie, Ross T.); Magdau, IB (Magdau, Ioan B.); Goncharov, AF (Goncharov, Alexander F.); Ackland, GJ (Ackland, Graeme J.); Gregoryanz, E (Gregoryanz, Eugene)

**Source:** PHYSICAL REVIEW LETTERS **Volume:** 113 **Issue:** 17 **Article Number:** 175501 **DOI:** 10.1103/PhysRevLett.113.175501 **Published:** OCT 21 2014

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**Record 48 of 57**

**Title:** Structural Properties of Nickel Dimethylglyoxime at High Pressure: Single-Crystal X-ray Diffraction and DFT Studies

**Author(s):** Bruce-Smith, IF (Bruce-Smith, Ian F.); Zakharov, BA (Zakharov, Boris A.); Stare, J (Stare, Jernej); Boldyreva, EV (Boldyreva, Elena V.); Pulham, CR (Pulham, Colin R.)

**Source:** JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 118 **Issue:** 42 **Pages:** 24705-24713 **DOI:** 10.1021/jp508939g **Published:** OCT 23 2014

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**Record 49 of 57****Title:** Ferrimagnetism in the High Pressure 6H-Perovskite BaCrO<sub>3</sub>**Author(s):** Arevalo-Lopez, AM (Arevalo-Lopez, Angel M.); Reeves, SJ (Reeves, Simon J.); Attfield, JP (Attfield, J. Paul)**Source:** ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE **Volume:** 640 **Issue:** 14 **Special Issue:** SI **Pages:** 2727-2729 **DOI:** 10.1002/zaac.201400353 **Published:** NOV 2014**Record 50 of 57****Title:** Approaching disorder-free transport in high-mobility conjugated polymers**Author(s):** Venkateshvaran, D (Venkateshvaran, Deepak); Nikolka, M (Nikolka, Mark); Sadhanala, A (Sadhanala, Aditya); Lemaur, V (Lemaur, Vincent); Zelazny, M (Zelazny, Mateusz); Kepa, M (Kepa, Michal); Hurhangee, M (Hurhangee, Michael); Kronemeijer, AJ (Kronemeijer, Auke Jisk); Pecunia, V (Pecunia, Vincenzo); Nasrallah, I (Nasrallah, Iyad); Romanov, I (Romanov, Igor); Broch, K (Broch, Katharina); McCulloch, I (McCulloch, Iain); Emin, D (Emin, David); Olivier, Y (Olivier, Yoann); Cornil, J (Cornil, Jerome); Beljonne, D (Beljonne, David); Sirringhaus, H (Sirringhaus, Henning)**Source:** NATURE **Volume:** 515 **Issue:** 7527 **Pages:** 384-388 **DOI:** 10.1038/nature13854 **Published:** NOV 20 2014**Record 51 of 57****Title:** Hard-soft synthesis of a new series of vacancy-ordered perovskites, CaCrO<sub>3</sub>-delta**Author(s):** Arevalo-Lopez, AM (Arevalo-Lopez, Angel M.); Liang, B (Liang, Bing); Senn, MS (Senn, Mark S.); Murray, C (Murray, Claire); Tang, C (Tang, Chiu); Attfield, JP (Attfield, J. Paul)**Source:** JOURNAL OF MATERIALS CHEMISTRY C **Volume:** 2 **Issue:** 44 **Pages:** 9364-9367 **DOI:** 10.1039/c4tc01808g **Published:** NOV 28 2014**Record 52 of 57****Title:** Symmetry-breaking 60 degrees-spin order in the A-site-ordered perovskite LaMn<sub>3</sub>V<sub>4</sub>O<sub>12</sub>**Author(s):** Saito, T (Saito, Takashi); Toyoda, M (Toyoda, Masayuki); Ritter, C (Ritter, Clemens); Zhang, SB (Zhang, Shoubao); Oguchi, T (Oguchi, Tamio); Attfield, JP (Attfield, J. Paul); Shimakawa, Y (Shimakawa, Yuichi)**Source:** PHYSICAL REVIEW B **Volume:** 90 **Issue:** 21 **Article Number:** 214405 **DOI:** 10.1103/PhysRevB.90.214405 **Published:** DEC 1 2014**Record 53 of 57****Title:** Incommensurate-to-incommensurate phase transition in Eu metal at high pressures**Author(s):** Husband, RJ (Husband, R. J.); Loa, I (Loa, I.); Munro, KA (Munro, K. A.); McBride, EE (McBride, E. E.); Evans, SR (Evans, S. R.); Liermann, HP (Liermann, H. -P.); McMahon, MI (McMahon, M. I.)**Source:** PHYSICAL REVIEW B **Volume:** 90 **Issue:** 21 **Article Number:** 214105 **DOI:** 10.1103/PhysRevB.90.214105 **Published:** DEC 8 2014**Record 54 of 57****Title:** Emergent transition for superconducting fluctuations in antiferromagnetic ruthenocuprates**Author(s):** McLaughlin, AC (McLaughlin, A. C.); Attfield, JP (Attfield, J. P.)**Source:** PHYSICAL REVIEW B **Volume:** 90 **Issue:** 22 **Article Number:** 220509 **DOI:** 10.1103/PhysRevB.90.220509 **Published:** DEC 15 2014**Record 55 of 57****Title:** Xenon Suboxides Stable under Pressure**Author(s):** Hermann, A (Hermann, Andreas); Schwerdtfeger, P (Schwerdtfeger, Peter)**Source:** JOURNAL OF PHYSICAL CHEMISTRY LETTERS **Volume:** 5 **Issue:** 24 **Pages:** 4336-4342 **DOI:** 10.1021/jz502230b **Published:** DEC 18 2014**Record 56 of 57****Title:** The crystal structure of methane B at 8 GPa-An alpha-Mn arrangement of molecules**Author(s):** Maynard-Casely, HE (Maynard-Casely, H. E.); Lundegaard, LF (Lundegaard, L. F.); Loa, I (Loa, I.); McMahon, MI (McMahon, M. I.); Gregoryanz, E (Gregoryanz, E.); Nelmes, RJ (Nelmes, R. J.); Loveday, JS (Loveday, J. S.)**Source:** JOURNAL OF CHEMICAL PHYSICS **Volume:** 141 **Issue:** 23 **Article Number:** 234313 **DOI:** 10.1063/1.4903813 **Published:** DEC 21 2014**Record 57 of 57****Title:** Incipient Ferromagnetism in Tb<sub>2</sub>Ge<sub>2</sub>O<sub>7</sub>: Application of Chemical Pressure to the Enigmatic Spin-Liquid Compound Tb<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>**Author(s):** Hallas, AM (Hallas, A. M.); Cheng, JG (Cheng, J. G.); Arevalo-Lopez, AM (Arevalo-Lopez, A. M.); Silverstein, HJ (Silverstein, H. J.); Su, Y (Su, Y.); Sarte, PM (Sarte, P. M.); Zhou, HD (Zhou, H. D.); Choi, ES (Choi, E. S.); Attfield, JP (Attfield, J. P.); Luke, GM (Luke, G. M.); Wiebe, CR (Wiebe, C. R.)**Source:** PHYSICAL REVIEW LETTERS **Volume:** 113 **Issue:** 26 **Article Number:** 267205 **DOI:** 10.1103/PhysRevLett.113.267205 **Published:** DEC 31 2014