

Daniel J. Frost – Publications in peer reviewed journals

2019

1. *Armstrong K, Frost DJ, McCammon CM, Rubie DC, Boffa-Ballaran T (2019) Deep magma ocean formation set the oxidation state of Earth's mantle. *Science* 365: 903-906.
2. Grüniger H, Liu Z, Siegel R, Boffa Ballaran T, Katsura T, Senker J, Frost DJ (2019) Oxygen vacancy ordering in aluminous bridgmanite in the Earth's lower mantle. *Geophysical Research Letters*, 46: 8731–8740.
3. Liu ZD, Ballaran TB, Huang R, Frost DJ, Katsura T (2019) Strong correlation of oxygen vacancies in bridgmanite with Mg/Si ratio. *Earth and Planetary Science Letters*, 523: UNSP 115697.
4. Liu ZD, Greaux S, Cai N, Siersch N, Boffa Ballaran T, Irifune T, Frost DJ, (2019) Influence of aluminum on the elasticity of majorite-pyrope garnets. *American Mineralogist*, 104: 929-935.
5. Elazar O, Frost D, Navon O, Kessel R (2019) Melting of H₂O and CO₂-bearing eclogite at 4-6 GPa and 900-1200 degrees C: Implications for the generation of diamond-forming fluids. *Geochimica et Cosmochimica Acta*, 255: 69-87.
6. Sinmyo R, Nakajima Y, McCammon C, Miyajima N, Petitgirard S, Myhill R, Dubrovinsky L, Frost DJ (2019) Effect of Fe³⁺ on Phase Relations in the Lower Mantle: Implications for Redox Melting in Stagnant Slabs. *Journal of Geophysical Research* doi: 10.1029/2019JB017704
7. Iizuka-Oku R, Soustelle V, Miyajima N, Walte NP, Frost DJ, Yagi T (2019) Experimentally deformed lawsonite at high pressure and high temperature: Implication for low velocity layers in subduction zones. *Physics of Earth and Planetary Interiors* 295: 106282, doi: 10.1016/j.pepi.2019.106282

2018

8. Sorbadere F, Laurenz V, Frost DJ, Wenz M, Rosenthal A, McCammon C, Rivard C (2018) The behaviour of ferric iron during partial melting of peridotite. *Geochimica et Cosmochimica Acta*, 239: 235-254.
9. Vogel AK, Jennings ES, Laurenz V, Rubie DC, Frost DJ (2018) The dependence of metal-silicate partitioning of moderately volatile elements on oxygen fugacity and Si contents of Fe metal: Implications for their valence states in silicate liquids *Geochimica et Cosmochimica Acta*, 237: 275-293.
10. Grüniger H, Schmutzler A, Siegel R, Armstrong K, Frost DJ, Senker J (2018) Quantitative description of H-1 SQ and DQ coherences for the hydroxyl disorder within hydrous ringwoodite. *Physical Chemistry Chemical Physics* 20: 15098-15105.
11. Yuan L, Ohtani E, Shibasaki Y, Ozawa S, Jin ZM, Suzuki A, Frost DJ (2018) The stability of anhydrous phase B, Mg₁₄Si₅O₂₄, at mantle transition zone conditions. *Physics and Chemistry of Minerals* 45: 523-531.
12. Pommier A, Laurenz V, Davies CJ, Frost DJ (2018) Melting phase relations in the Fe-S and Fe-S-O systems at core conditions in small terrestrial bodies. *Icarus* 306: 150-162.
13. Comboni D, Lotti P, Gatta GD, Merlini M, Liermann HP, Frost DJ (2018) Pargasite at high pressure and temperature. *Physics and Chemistry of Minerals*, 45: 259-278.

14. Uenver-Thiele L, Woodland AB, Miyajima N, Ballaran TB, Frost DJ (2018) Behaviour of Fe_4O_5 - $\text{Mg}_2\text{Fe}_2\text{O}_5$ solid solutions and their relation to coexisting Mg-Fe silicates and oxide phases. *Contributions to Mineralogy and Petrology* 173: doi: 10.1007/s00410-018-1443-8.
15. Beyer C, Rosenthal A, Myhill R, Crichton WA, Yu T, Wang YB, Frost DJ (2018) An internally consistent pressure calibration of geobarometers applicable to the Earth's upper mantle using in situ XRD. *Geochimica et Cosmochimica Acta*, 222: 421-435.

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16. Uenver-Thiele L, Woodland AB, Ballaran TB, Miyajima N, Frost DJ (2017) Phase relations of Fe-Mg spinels including new high-pressure post-spinel phases and implications for natural samples. *American Mineralogist*, 102: 2054-2064.
17. Farla R, Rosenthal A, Bollinger C, Petitgirard S, Guignard J, Miyajima N, Kawazoe T, Crichton, WA, Frost DJ (2017) High-pressure, high-temperature deformation of dunite, eclogite, clinopyroxenite and garnetite using in situ X-ray diffraction. *Earth and Planetary Science Letters*, 473: 291-302.
18. Novella D, Dolejs D, Myhill R, Pamato MG, Manthilake G, Frost DJ (2017) Melting phase relations in the systems Mg_2SiO_4 - H_2O and MgSiO_3 - H_2O and the formation of hydrous melts in the upper mantle. *Geochimica et Cosmochimica Acta*, 204: 68-82.
19. Posner ES, Rubie DC, Frost DJ, Vlcek V, Steinle-Neumann G (2017) High P-T experiments and first principles calculations of the diffusion of Si and Cr in liquid iron. *Geochimica et Cosmochimica Acta*, 203: 323-342.
20. Posner ES, Rubie DC, Frost DJ, Steinle-Neumann G (2017) Experimental determination of oxygen diffusion in liquid iron at high pressure. *Earth and Planetary Science Letters*, 464:116-123.
21. Myhill R, Frost DJ, Novella D (2017) Hydrous melting and partitioning in and above the mantle transition zone: Insights from water-rich MgO-SiO_2 - H_2O experiments. *Geochimica et Cosmochimica Acta*, 200: 408-421.
22. *Kurnosov A, Marquardt H, Frost DJ, Boffa Ballaran T, Ziberna L (2017) Evidence for a Fe^{3+} -rich lower mantle from Al-Fe-bridgmanite elasticity data. *Nature*, 543: 543-546.
23. Laumonier M, Farla R, Frost DJ, Katsura T, Marquardt K, Bouvier AS, Baumgartner LP (2017) Experimental determination of melt interconnectivity and electrical conductivity in the upper mantle. *Earth and Planetary Science Letters*, 463: 286-297.
24. Uenver-Thiele L, Woodland AB, Ballaran TB, Miyajima N, Frost DJ (2017) Phase relations of MgFe_2O_4 at conditions of the deep upper mantle and transition zone. *American Mineralogist*, 102: 632-642.
25. Beyer C, Frost DJ (2017) The depth of sub-lithospheric diamond formation and the redistribution of carbon in the deep mantle. *Earth and Planetary Science Letters*, 461: 30-39.
26. Gruninger H, Armstrong K, Greim D, Boffa-Ballaran T, Frost DJ, Senker J (2017) Hidden oceans? Unraveling the structure of hydrous defects in the Earth's deep interior. *Journal of the American Chemical Society*, 139: 10499-10505.

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27. Laurenz V, Rubie DC, Frost DJ, Vogel AK (2016) The importance of sulfur for the behavior of highly-siderophile elements during Earth's differentiation. *Geochimica et Cosmochimica Acta*, 194: 123-138.

28. Bureau H, Frost DJ, Bolfan-Casanova N, Leroy C, Esteve I, Cordier P (2016) Diamond growth in mantle fluids. *Lithos*, 265, 4-15.
29. Konyashin I, Frost DJ, Crossley A, Jurkschat K, Johnston C, Armstrong K (2016) Nano-diamond obtained from adipic acid at ultra-high pressures. *Materials Letters*, 183: 14-18.
30. Pamato MG, Kurnosov A, Ballaran TB, Frost DJ, Ziberna L, Giannini M, Speziale S, Tkachev SN, Zhuravlev KK, Prakapenka VB (2016) Single crystal elasticity of majoritic garnets: Stagnant slabs and thermal anomalies at the base of the transition zone. *Earth and Planetary Science Letters*, 451: 114-124.
31. Rubie DC, Laurenz V, Jacobson SA, Morbidelli A, Palme H, Vogel AK, Frost DJ (2016) Highly siderophile elements were stripped from Earth's mantle by iron sulfide segregation. *Science*, 353: 1141-1144.
32. Kempl J, Vroon PZ, van der Wagt B, Zinngrebe E, Frost DJ, van Westrenen W (2016) Silicon stable isotope fractionation between metal and silicate at high-pressure, high-temperature conditions as a tracer of planetary core formation. *Netherlands Journal of Geosciences*, 95: 113-129.
33. Myhill R, Ojwang DO, Ziberna L, Frost DJ, Ballaran TB, Miyajima N (2016) On the P-T f_{O_2} stability of Fe_4O_5 , Fe_5O_6 and Fe_4O_5 -rich solid solutions. *Contributions to Mineralogy and Petrology*, 171, Article Number: 151 DOI: 10.1007/s00410-016-1258-4.
34. Chantel J, Manthilake GM, Frost DJ, Beyer C, Ballaran TB, Jing ZC, Wang YB (2016) Elastic wave velocities in polycrystalline $Mg_3Al_2Si_3O_{12}$ -pyrope garnet to 24 GPa and 1300 K. *American Mineralogist*, 101: 991-997.

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35. Fischer RA, Nakajima Y, Campbell AJ, Frost DJ, Harries D, Langenhorst F, Miyajima N, Pollok K, Rubie DC (2015) High pressure metal-silicate partitioning of Ni, Co, V, Cr, Si, and O. *Geochimica et Cosmochimica Acta*, 167, 177-194.
36. Serghiou G, Ji G, Odling N, Reichmann HJ, Morniroli JP, Boehler R, Frost DJ, Wright JP, Wunder B (2015) Creating reactivity with unstable endmembers using pressure and temperature: synthesis of bulk cubic $Mg_{0.4}Fe_{0.6}N$. *Angewandte Chemie-International Edition*, 54: 15109-15112.
37. Chang YY, Jacobsen SD, Bina CR, Thomas SM, Smyth JR, Frost DJ, Ballaran TB, McCammon, CA, Hauri EH, Inoue T, Yurimoto H, Meng Y, Dera P (2015) Comparative compressibility of hydrous wadsleyite and ringwoodite: Effect of H_2O and implications for detecting water in the transition zone. *Journal of Geophysical Research- Solid Earth*, 120: 8259-8280.
38. Roberge M, Bureau H, Bolfan-Casanova N, Frost DJ, Raepsaet C, Surble S, Khodja H, Auzende AL, Fiquet G (2015) Is the transition zone a deep reservoir for fluorine? *Earth and Planetary Science Letters*, 429: 25-32.
39. King SD, Frost DJ, Rubie DC (2015) Why cold slabs stagnate in the transition zone. *Geology*, 43: 231-234.
40. Beyer C, Frost DJ, Miyajima N (2015) Experimental calibration of a garnet-clinopyroxene geobarometer for mantle eclogites. *Contributions to Mineralogy and Petrology*, 169: 18 DOI: 10.1007/s00410-015-1113-z.
41. Stagno V, Frost DJ, McCammon CA, Mohseni H, Fei Y (2015) The oxygen fugacity at which graphite or diamond forms from carbonate-bearing melts in eclogitic rocks. *Contributions to Mineralogy and Petrology*, 169: 16 DOI: 10.1007/s00410-015-1111-1.

42. Auzende AL, Escartin J, Walte NP, Guillot S, Hirth G, Frost DJ (2015) Deformation mechanisms of antigorite serpentinite at subduction zone conditions determined from experimentally and naturally deformed rocks. *Earth and Planetary Science Letters*, 411: 229-240.
43. Serghiou G, Ji G, Odling N, Reichmann HJ, Frost DJ, Wright JP (2015) Synthesis and high-resolution study distinguishing between very similar interstitial iron nitride structures. *High Pressure Research*, 35: 28-36.
44. Rubie DC, Jacobson SA, Morbidelli A, O'Brien DP, Young ED, de Vries J, Nimmo F, Palme H, Frost DJ (2015) Accretion and differentiation of the terrestrial planets with implications for the compositions of early-formed Solar System bodies and accretion of water. *Icarus*, 248: 89–108.
45. *Pamato MG, Myhill R, Boffa Ballaran T, Frost DJ, Heidelbach F, Miyajima N (2015) Lower-mantle water reservoir implied by the extreme stability of a hydrous aluminosilicate. *Nature Geoscience*, 8: 75–79.

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46. Novella D, Frost DJ (2014) The composition of hydrous partial melts of garnet peridotite at 6 GPa: Implications for the origin of group II kimberlites. *Journal of Petrology*, 55: 2097-2123.
47. Novella D, Frost DJ, Hauri EH, Bureau H, Raepsaet C, Roberge M (2014) The distribution of H₂O between silicate melt and nominally anhydrous peridotite and the onset of hydrous melting in the deep upper mantle. *Earth and Planetary Science Letters*, 400: 1-13.
48. Pamato MG, Kurnosov A, Ballaran TB, Trots DM, Caracas R, Frost DJ (2014) Hexagonal Na_{0.41}[Na_{0.125}Mg_{0.79}Al_{0.085}]₂[Al_{0.79}Si_{0.21}]₆O₁₂ (NAL phase): Crystal structure refinement and elasticity. *American Mineralogist*, 99: 1562-1569.
49. Glazyrin K, Ballaran TB, Frost DJ, McCammon C, Kantor A, Merlini, Hanfland M, Dubrovinsky L (2014) Magnesium silicate perovskite and effect of iron oxidation state on its bulk sound velocity at the conditions of the lower mantle. *Earth and Planetary Science Letters*, 393: 182-186.
50. Soustelle V, Walte NP, Manthilake MAGM, Frost DJ (2014) Melt migration and melt-rock reactions in the deforming Earth's upper mantle: Experiments at high pressure and temperature. *Geology*, 42: 83-86.

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51. Woodland AB, Schollenbruch K, Koch M, Ballaran TB, Angel RJ, Frost DJ (2013) Fe₄O₅ and its solid solutions in several simple systems. *Contributions to Mineralogy and Petrology*, 166: 1677-1686.
52. Shirey SB, Cartigny P, Frost DJ, Keshav S, Nestola F, Nimis P, Pearson DG, Sobolev NV, Walter MJ (2013) Diamonds and the geology of mantle carbon. *Reviews in Mineralogy & Geochemistry*, 75: 355-421.
53. Chang YY, Jacobsen SD, Lin JF, Bina CR, Thomas SM, Wu JJ, Shen GY, Xiao YM, Chow P, Frost DJ, McCammon CA, Dera P (2013) Spin transition of Fe³⁺ in Al-bearing phase D: An alternative explanation for small-scale seismic scatterers in the mid-lower mantle. *Earth and Planetary Science Letters*, 382, 1-9.
54. Trots DM, Kurnosov A, Ballaran TB, Tkachev S, Zhuravlev K, Prakapenka V, Berkowski M, Frost DJ (2013) The Sm:YAG primary fluorescence pressure scale. *Journal of Geophysical Research- Solid Earth*, 118: 5805-5813.
55. Manghnani MH, Hushur A, Smyth JR, Nestola F, Dera P, Sekar M, Amulele G, Frost DJ (2013) Compressibility and structural stability of two variably hydrated olivine samples (Fo(97)Fa(3)) to 34 GPa by X-ray diffraction and Raman spectroscopy. *American Mineralogist*, 98: 1972-1979.

56. Trots DM, Kurnosov A, Manthilake MAGM, Ovsyannikov SV, Akselrud LG, Hansen T, Smyth JR, Frost DJ (2013) The determination of hydrogen positions in superhydrous phase B. *American Mineralogist*, 98: 1688-1692.
57. Mussi A, Cordier P, Frost, DJ (2013) Transmission electron microscopy characterization of the dislocations and slip systems of the dense hydrous magnesium silicate superhydrous B. *European Journal of Mineralogy*, 25: 561-568.
58. van Mierlo WL, Langenhorst F, Frost DJ, Rubie DC (2013) Stagnation of subducting slabs in the transition zone due to slow diffusion in majoritic garnet. *Nature Geoscience*, 6: 400-403.
59. Manthilake MAGM, Miyajima N, Heidelbach F, Soustelle V, Frost DJ (2013) The effect of aluminum and water on the development of deformation fabrics of orthopyroxene. *Contributions to Mineralogy and Petrology*, 165: 495-505.
60. Panero WR, Smyth JR, Pigott JS, Liu ZX, Frost DJ (2013) Hydrous ringwoodite to 5 K and 35 GPa: Multiple hydrogen bonding sites resolved with FTIR spectroscopy. *American Mineralogist*, 98: 637-642.
61. Tsuno K, Frost DJ, Rubie DC (2013) Simultaneous partitioning of silicon and oxygen into the Earth's core during early Earth differentiation. *Geophysical Research Letters*, 40: 66-71.
62. *Stagno V, Ojwang DO, McCammon CA, Frost DJ (2013) The oxidation state of the mantle and the extraction of carbon from Earth's interior. *Nature*, 493: 84-88.
63. Griffin JM, Berry AJ, Frost DJ, Wimperis S, Ashbrook SE (2013) Water in the Earth's mantle: a solid-state NMR study of hydrous wadsleyite. *Chemical Science*, 4: 1523-1538.

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64. Woodland AB, Frost DJ, Trots DM, Klimm K, Mezouar M (2012) In situ observation of the breakdown of magnetite (Fe_3O_4) to Fe_4O_5 and hematite at high pressures and temperatures. *American Mineralogist*, 97:1808-1811.
65. Chantel J, Mookherjee M, Frost DJ (2012) The elasticity of lawsonite at high pressure and the origin of low velocity layers in subduction zones. *Earth and Planetary Science Letters*, 349: 116-125.
66. Williams HM, Wood BJ, Wade J, Frost DJ, Tuff J (2012) Isotopic evidence for internal oxidation of the Earth's mantle during accretion. *Earth and Planetary Science Letters*, 321: 54-63.
67. Posner ES, Konzett J, Frost DJ, Downs RT, Yang HX (2012) High-pressure synthetic $(\text{Na}_{0.97}\text{Mg}_{0.03})(\text{Mg}_{0.43}\text{Fe}_{0.173}\text{Si}_{0.40})\text{Si}_2\text{O}_6$, with six-coordinated silicon, isostructural with P2/n omphacite. *Acta Crystallographica Section E- Structure Reports Online*, 68, I18-U166 DOI: 10.1107/S1600536812002966.
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69. Bureau H, Langenhorst F, Auzende AL, Frost DJ, Esteve I, Siebert J (2012) The growth of fibrous, cloudy and polycrystalline diamonds. *Geochimica et Cosmochimica Acta*, 77: 202-214.
70. Smyth JR, Miyajima N, Huss GR, Hellebrand E, Rubie DC, Frost DJ (2012) Olivine-wadsleyite-pyroxene topotaxy: Evidence for coherent nucleation and diffusion-controlled growth at the 410-km discontinuity. *Physics of Earth and Planetary Interiors*, 200: 85-91.

71. Manthilake MAGM, Walte N, Frost DJ (2012) A new multi-anvil press employing six independently acting 8 MN hydraulic rams. *High Pressure Research*, 32: 195-207.
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74. Ballaran TB, Kurnosov A, Glazyrin K, Frost DJ, Merlini M, Hanfland M, Caracas R (2012) Effect of chemistry on the compressibility of silicate perovskite in the lower mantle. *Earth and Planetary Science Letters*, 333: 181-190.
75. Mao Z, Lin JF, Jacobsen SD, Duffy TS, Chang YY, Smyth JR, Frost DJ, Hauri EH, Prakapenka VB (2012) Sound velocities of hydrous ringwoodite to 16 GPa and 673 K. *Earth and Planetary Science Letters*, 331: 112-119.
76. Mussi A, Cordier P, Frost DJ (2012) Crystal defects in dense hydrous magnesium silicate phase A deformed at high pressure: characterization by transmission electron microscopy. *European Journal of Mineralogy*, 24: 429-438.
77. Welch MD, Konzett J, Bindi L, Kohn SC, Frost DJ (2012) New structural features of the high-pressure synthetic sheet-disilicate Phase-X, K_(2-x)Mg₂Si₂O₇H_x. *American Mineralogist*, 97: 1849-1857.
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79. Chantel J, Frost DJ, McCammon CA, Jing ZC, Wang YB (2012) Acoustic velocities of pure and iron-bearing magnesium silicate perovskite measured to 25 GPa and 1200 K. *Geophysical Research Letters*, 39 L19307 DOI:10.1029/2012GL053075.
80. Trots DM, Kurnosov A, Ballaran TB, Frost DJ (2012) High-temperature structural behaviors of anhydrous wadsleyite and forsterite. *American Mineralogist*, 97: 1582-1590.
81. Mann U, Frost DJ, Rubie DC, Becker H, Audetat A (2012) Partitioning of Ru, Rh, Pd, Re, Ir and Pt between liquid metal and silicate at high pressures and high temperatures: Implications for the origin of highly siderophile element concentrations in the Earth's mantle. *Geochimica et Cosmochimica Acta*, 84: 593-613.
82. Ye Y, Brown DA, Smyth JR, Panero WR, Jacobsen SD, Chang YY, Townsend JP, Thomas SM, Hauri EH, Dera P, Frost DJ (2012) Compressibility and thermal expansion of hydrous ringwoodite with 2.5(3) wt% H₂O. *American Mineralogist*, 97: 573-582.

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85. Rubie DC, Frost DJ, Mann U, Asahara Y, Nimmo F, Tsuno K, Kegler P, Holzheid A, Palme H (2011) Heterogeneous accretion, composition and core-mantle differentiation of the Earth. *Earth and Planetary Science Letters*, 301 (1-2): 31-42.

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97. Irifune T, Shinmei T, McCammon CA, Miyajima N, Rubie DC, Frost DJ (2010) Iron Partitioning and Density Changes of Pyrolite in Earth's Lower Mantle. *Science*, 327: 193-195.
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