

Nancy L. Ross Publications

Department of Geosciences
Virginia Polytechnic Institute & State University
Blacksburg, VA 24061, USA
Tel: (+1)540-231-6356; Fax: (+1)540-231-3386
Email: nross@vt.edu

ARTICLES:

- [1] **Ross N.L.** and Meagher E.P. (1984) A molecular orbital study of $H_6Si_2O_7$ under simulated compression. American Mineralogist 69: 1145-1149.
- [2] **Ross N.L.** and McMillan P. (1984) The Raman spectrum of $MgSiO_3$ ilmenite. American Mineralogist 69: 719-721.
- [3] Akaogi M., **Ross N.L.**, McMillan P., and Navrotsky A. (1984) The Mg_2SiO_4 Polymorphs (olivine, modified spinel and spinel) - thermodynamic properties from oxide melt solution calorimetry, phase relations, and models of lattice vibrations. American Mineralogist 69: 499-512.
- [4] **Ross N.L.**, Akaogi M., Navrotsky A., Susaki J., and McMillan P. (1986) Phase transitions among the $CaGeO_3$ polymorphs (wollastonite, garnet, and perovskite structures): Studies by high-pressure synthesis, high-temperature calorimetry, and vibrational spectroscopy and calculation. Journal of Geophysical Research 91: 4685-4696.
- [5] McKelvey M.J., O'Bannon G.W., Larson E.M., Marzke R.F., Eckert J., and **Ross N.L.** (1986) Synthesis, characterization and properties of the new ionic intercalation compound $(NH_4^+)^{0.22}TiS_2^{0.22-}$. Materials Research Bulletin 21: 1323-1333.
- [6] McMillan P.F. and **Ross N.L.** (1987) Heat capacity calculations for Al_2O_3 corundum and $MgSiO_3$ ilmenite. Physics and Chemistry of Minerals 14: 225-234.
- [7] **Ross N.L.** and Navrotsky A. (1987) The Mg_2GeO_4 olivine - spinel phase transition. Physics and Chemistry of Minerals 14: 473-481.
- [8] Geisinger K.L., **Ross N.L.**, McMillan P., and Navrotsky A. (1987) $K_2Si_4O_9$: Energetics and vibrational spectra of glass, sheet, and wadeite-type phases. American Mineralogist 72: 984-994.
- [9] Hazen R.M., Finger L.W., Angel R.J., Prewitt C.T., **Ross N.L.**, Mao H.K., Hadidiacos C.G., Hor P.H., Meng R.L., and Chu C.W. (1987) Crystallographic description of the phases in the Y-Ba-Cu-O superconductor. Physical Review B35:7238-7241.

- [10] Hazen R.M., Prewitt C.T., Angel R.J., **Ross N.L.**, Finger L.W., Hadidiacos C.G., Veblen D.R., Heaney P.J., Hor P.H., Meng R.L., Sun Y.Y., Wang Y.Q., Xue Y.Y., Huang Z.J., Gao L., Bechtold J., and Chu C.W. (1988) Superconductivity in the very high T_c Bi-Ca-Sr-Cu-O system: Phase identification. Physics Review Letters 60:1174-1177.
- [11] Meng R.L., Hor P.H., Sun Y.Y., Huang Z.J., Gao L., Xue Y.Y., Wang Y.Q., Bechtold J., Chu C.W., Hazen R.M., Prewitt C.T., Angel R.J., **Ross N.L.**, Finger L.W., and Hadidiacos C.G. (1988) The 120K superconducting phase in Bi-Ca-Sr-Cu-O. Modern Physics Letters 2:543-549.
- [12] Veblen D.R., Heaney P.J., Angel R.J., Finger L.W., Hazen R.M., Prewitt C.T., **Ross N.L.**, Chu C.W., Hor P.H., and Meng R.L. (1988) Crystallography, chemistry, and structural disorder in the new high- T_c Bi-Ca-Sr-Cu-O superconductor. Nature, 332:334-337.
- [13] Hazen R.M., Finger L.W., Angel R.J., Prewitt C.T., **Ross N.L.**, Hadidiacos C.G., Heaney P.J., Veblen D.R., Sheng V.V., Ali A.E., and Hermann A.M. (1988) 100K superconducting phases in the Tl-Ca-Ba-Cu-O system. Physics Review Letters 60:1657-1660.
- [14] Angel R.J., Gasparik T., **Ross N.L.**, Finger L.W., Prewitt C.T., and Hazen R.M. (1988) A silica-rich sodium pyroxene phase with six-coordinated silicon. Nature, 333:156-158.
- [15] Angel R.J., and **Ross N.L.** (1988) The I-1 to P-1 transition in anorthite-rich feldspars. Annual Report of the Director of the Geophysical Laboratory, Carnegie Institution of Washington, 91-95.
- [16] Hazen R.M., Finger L.W., Angel R.J., **Ross N.L.**, Prewitt C.T., Mao H.K., Hadidiacos C.G., George D.J., Veblen D.R., and Heaney P.J. (1988) Superconductivity in new high- T_c systems: Phase identification. Annual Report of the Director of the Geophysical Laboratory, Carnegie Institution of Washington, 99-106.
- [17] McMillan P. and **Ross N.L.** (1988) The Raman spectra of several orthorhombic calcium oxide perovskites. Physics and Chemistry of Minerals 16: 21-28.
- [18] **Ross N.L.** and Navrotsky A. (1988) Study of the $MgGeO_3$ polymorphs (orthopyroxene, clinopyroxene, and ilmenite structures) by calorimetry, spectroscopy, and phase equilibria. American Mineralogist 73: 1355-1365.
- [19] **Ross N.L.** and Hazen R.M. (1989) Single crystal X-ray diffraction study of $MgSiO_3$ perovskite from 77 to 400 K. Physics and Chemistry of Minerals 16: 415-420.
- [20] **Ross N.L.**, Ko J., and Prewitt C.T. (1989) A new phase transition in $MnTiO_3 : LiNbO_3$ to perovskite structure. Physics and Chemistry of Minerals 16: 621-629.
- [21] Angel R.J., Redfern S.A.T., and **Ross N.L.** (1989) Spontaneous strain below the I-1→P-1 transition in anorthite at pressure. Physics and Chemistry of Minerals, 16:539-544.

- [22] **Ross N.L.**, and Leinenweber K. (1990) Single crystal structure refinement of high-pressure ZnGeO₃ ilmenite. Zeitschrift fur Kristallographie 191:93-104.
- [23] Prewitt C.T., Ko J., and **Ross N.L.** (1990) High pressure, single crystal studies of MnTiO₃. High Pressure Research 4:426-428.
- [24] **Ross N.L.**, Shu J., Hazen R.M., and Gasparik T. (1990) High pressure crystal chemistry of stishovite. American Mineralogist 75:739-747.
- [25] **Ross N.L.**, and Hazen R.M. (1990) High pressure crystal chemistry of MgSiO₃ perovskite. Physics and Chemistry of Minerals 17: 228-237.
- [26] Angel R.J., **Ross N.L.**, Finger L.W., and Hazen R.M. (1990) Ba₃CaCuSi₆O₁₇: A new **IB**{1¹_∞} [⁴Si₆O₁₇] chain silicate. Acta Crystallographica C46, 2028-2030.
- [27] **Ross N.L.**, and Angel R.J. (1991) Crystal structure of high-pressure SrB₂O₄ (IV). Journal of Solid State Chemistry 90:27-30.
- [28] **Ross N.L.**, Reynard B., and Guyot F. (1991) Crystal structure of high-pressure MnGeO₃ ilmenite. Acta Crystallographica, C47:1794-1796.
- [29] **Ross N.L.** and Reeder R.J. (1992) High pressure structural study of dolomite and ankerite. American Mineralogist, 77:412-421.
- [30] Angel R.J., **Ross N.L.**, and Wood I.G. (1992) Single crystal X-ray diffraction at high pressure. Phase Transitions, 39: 13-32.
- [31] Angel R.J., Chopelas A., and **Ross N.L.** (1992) Stability of high-density clinoenstatite at upper-mantle pressures. Nature, 358: 322-324.
- [32] **Ross N.L.**, Reynard B., and Guyot F. (1992) High pressure structural study of MnGeO₃ ilmenite. Zeitschrift fur Kristallographie, 204, 43-55.
- [33] **Ross N.L.** (1992) Fourier transform Raman spectroscopy at high pressures: Preliminary results of sulphur to 56 Kbar. Spectrochimica Acta, 49A, 681-684.
- [34] Hayward C., Angel R.J., **Ross N.L.** (1994) The structural redetermination and crystal chemistry of sinhalite, MgAlBO₄. European Journal of Mineralogy, 6, 313-321.
- [35] Hayward C., Best S.R. , **Ross N.L.**, Clark R., and Witnall R. (1994) Polarised single crystal Raman spectroscopy of sinhalite, MgAlBO₄, Spectrochimica Acta, 50A, 1287-1294.
- [36] Wentzcovitch R., **Ross N.L.**, and Price,G.D. (1995) An ab-initio study of MgSiO₃ and CaSiO₃ perovskites at lower mantle pressures, Physics of Earth and Planetary Interiors, 90, 101-112.

- [37] **Ross N.L.** (1996) Distortions in GdFeO₃-type perovskites with pressure: A study of YAlO₃ to 5 GPa. *Phase Transitions*, 58, 27-41.
- [38] Sowerby J.R. and **Ross N.L.** (1996) Electronic absorption spectra of clinoferrosilite to 5 GPa, *Physics and Chemistry of Minerals*, 23, 297.
- [39] Angel R.J., **Ross N.L.**, Seifert F. and Fliervoet T.F. (1996) Structural characterization of pentacoordinate silicon in a calcium silicate. *Nature*, 384, 441-444.
- [40] **Ross N.L.** (1997) The equation of state and high-pressure behaviour of magnesite. *American Mineralogist*, 82, 682-688.
- [41] **Ross N.L.** (1997) Optical absorption spectra of transition zone minerals and implications for radiative heat transport. *Physics and Chemistry of the Earth*, 22, 113-118.
- [42] Angel, R.J. and **Ross, N.L.** (1997) Equations of state of mantle minerals from high-pressure diffraction. *Physics and Chemistry of the Earth*, 22, 119-123.
- [43] Chaplin T., Price G.D., and **Ross N.L.** (1998) Computer simulation of the infrared and Raman activity of pyrope garnet, and assignment of calculated modes to specific atomic motions. *American Mineralogist*, 83, 841-847.
- [44] **Ross N.L.** (1998) High pressure study of ScAlO₃ perovskite. *Physics and Chemistry of Minerals*, 25, 597-602.
- [45] Chakraborty S., Knoche R., Schulze H., Rubie D.C., Dobson D., **Ross N.L.**, and Angel R.J. (1999) Enhancement of cation diffusion rates across the 410-km discontinuity in the Earth's Mantle. *Science*, 283, 362-365.
- [46] **Ross N.L.** and Angel R.J. (1999) Compression of CaTiO₃ and CaGeO₃ perovskites. *American Mineralogist*, 84, 277-281.
- [47] **Ross N.L.** and Reynard B. (1999) The effect of Fe²⁺ on the P2₁/c to C2/c transition in (Mg,Fe)SiO₃ clinopyroxenes. *European Journal of Mineralogy*, 11, 585-589.
- [48] Crichton W.A., **Ross N.L.**, and Gasparik T. (1999) Equations of state of Anhydrous B and Superhydrous-B. *Physics and Chemistry of Minerals*, 26, 570-575.
- [49] **Ross N.L.** and Sowerby J.R. (1999) High-pressure crystal field spectra of single crystal clinoferrosilite. *European Journal of Mineralogy*, 11, 791-801.
- [50] Chaplin T.D., **Ross N.L.** and Reynard B. (2000) A high-temperature and high-pressure Raman spectroscopic study of CaGeO₃ garnet. *Physics and Chemistry of Minerals*, 27, 213-219.

- [51] Crichton W.A. and **Ross N.L.** (2000) Equation of state of phase E. *Mineralogical Magazine*, 64, 561-567.
- [52] Crichton W.A. and **Ross N.L.** (2000) Single crystal equation of state measurements on Mg-End-Members of the B-group Minerals. In: M.H. Manghnani, W.J. Nellis and M.F. Nicol (Eds), AIRAPT-17 Proceedings - Science and Technology of High Pressure , Volume II, pp 587-590. Universities Press, Hyderabad, India.
- [53] Kung J., Angel R.J. and **Ross N.L.** (2001) Elasticity of CaSnO_3 perovskite. *Physics and Chemistry of Minerals*, 28:35-43.
- [54] Schoenitz M., Navrotsky A., and **Ross N.L.** (2001) Enthalpy of formation of CaSi_2O_5 , a quenched high-pressure phase with pentacoordinate silicon. *Physics and Chemistry of Minerals*, 28: 57-60.
- [55] Boffa-Ballaran T., Carpenter M.A., and **Ross N.L.** (2001) Infrared-powder absorption spectroscopy of Ca-free $\text{P}_2\text{l/c}$ clinopyroxenes. *Mineralogical Magazine*, 65:339-350.
- [56] Angel R.J., Frost D.J., **Ross N.L.** and Hemley R.J. (2001) Stabilities and EoS of dense hydrous magnesium silicates. *Physics of Earth and Planetary Interiors*, 127:181-196
- [57] **Ross N.L.** and Crichton W.A. (2001) Compression of hydroxy-clinohumite ($\text{Mg}_9\text{Si}_4\text{O}_{16}(\text{OH})_2$) and hydroxy-chondrodite ($\text{Mg}_5\text{Si}_2\text{O}_8(\text{OH})_2$). *American Mineralogist*, 86, 990-996.
- [58] Le Godec, Y., Dove M.T., Francis D.J., Kohn S.C., Marshall W.G., Pawley A.R., Price G.D., Redfern S.A.T., Rhodes N., **Ross N.L.**, Schofield P.F., Schoonveld E., Syfosse G., Tucker M.G., and Welch M.D. (2001) Neutron diffraction of simultaneous high temperatures and pressures, with measurement of temperature by neutron radiography. *Mineralogical Magazine*, 65, 737-748.
- [59] Kleppe, A., Jephcoat, A.P., and **Ross, N.L.** (2001) Raman spectroscopic studies of Phase E to 19 GPa. *American Mineralogist*, 86, 1275-1281.
- [60] Welch, M.D., Marshall W.G., **Ross, N.L.**, and Knight, K.S. (2001) Hydrogen positions in leucophoenicite , $\text{Mn}_7\text{Si}_3\text{O}_{12}(\text{OH})_2$: A close relative of the hydrous B phases. *American Mineralogist*, 87, 154-159.
- [61] Crichton, W.A. and **Ross, N.L.** (2002) Equation of state of dense hydrous magnesium silicate phase A, $\text{Mg}_7\text{Si}_2\text{O}_8(\text{OH})_6$. *American Mineralogist*, 87, 333-338 .
- [62] **Ross, N.L.**, Angel, R.J. and Seifert, F. (2002) Compressibility of Brownmillerite, $\text{Ca}_2\text{Fe}_2\text{O}_5$: Effect of Vacancies on the Elastic Properties of Perovskites. *Physics of Earth and Planetary Interiors*, 129, 145-151.

- [63] **Ross, N.L.**, Chaplin T.D. and Welch, M.D. (2002) Compressibility of Stottite, FeGe(OH)₆: An octahedral framework with protonated oxygens. *American Mineralogist*, 87, 1410-114.
- [64] **Ross, N.L.**, Angel, R.J., Chaplin, T.D. and Kung, J.(2002) Elastic Properties of Ca-perovskites. *Materials Research Society Symposium Proceedings*, 718, 115-119.
- [65] McCammon C.A., and **Ross N.L.** (2003) Crystal chemistry of ferric iron in (Mg,Fe,Al)SiO₃ majorite with implications for the transition zone. *Physics and Chemistry of Minerals*, 30, 206-216.
- [66] **Ross, N.L.** and Chaplin, T.D. (2003) Compressibility of CaZrO₃ perovskite: Comparison with Ca-oxide perovskites. *Journal of Solid State Chemistry*, 172, 123-126.
- [67] **Ross N.L.**, Gibbs, G.V., and Rosso, K.M. (2003) Potential docking sites and positions of hydrogen in high-pressure silicates, *American Mineralogist*, 88, 1452-1459.
- [68] Liu Z., Lager G.S., Hemley R.J. and **Ross N.L.** (2003) Synchrotron infrared spectroscopy of OH-chondrodite and OH-clinohumite at high pressure. *American Mineralogist*, 88, 1412-1415
- [69] Gibbs G.V., Cox D.E., Boisen, M.B. Jr., Downs R.T., and **Ross N.L.** (2003) The electron localization function: A tool for locating favorable proton docking sites in the silica polymorphs. *Physics and Chemistry of minerals*, 30, 305-316.
- [70] Gibbs G.V., Cox D.F., and **Ross N.L.** (2004) A modeling of favorable H-docking sites and defects in the high pressure silica polymorph stishovite. *Physics and Chemistry of Minerals*, 31:232-239.
- [71] Zhao J., **Ross N.L.** and Angel R.J. (2004) Tilting and distortion of CaSnO₃ perovskite to 7 GPa determined from single-crystal X-ray diffraction. *Physics and Chemistry of Minerals*, 31:299-305
- [72] **Ross N.L.**, Zhao J., and Angel R.J. (2004) High-pressure single-crystal X-ray diffraction study of YAlO₃ perovskite. *Journal of Solid State Chemistry*, 177:1276-1284.
- [73] Zhao J., **Ross, N.L.** and Angel,R.J. (2004) A new view of the high-pressure behaviour of GdFeO₃-type perovskites. *Acta Crystallographica B*, B60: 263-271.
- [74] McCammon C.A., Frost D.J., Smyth J.R., Laustsen H.M.S., Kawamoto T., **Ross N.L.**, van Aken P.A. (2004) Oxidation state of iron in hydrous mantle phases: implications for subduction and mantle oxygen fugacity. *Physics of the Earth and Planetary Interiors* 143-44: 157-169.
- [75] **Ross N.L.**, Zhao J., Burt J.B., and Chaplin T.D. (2004) Equations of state of GdAlO₃ and GdFeO₃ perovskites. *Journal of Physics: Condensed Matter*, 16: 5721-5731.
- [76] **Ross N.L.**, Zhao J., and Angel R.J. (2004) High-pressure structural behavior of GdAlO₃ and GdFeO₃ perovskites *Journal of Solid State Chemistry*, 172, in press.

BOOK CHAPTERS:

- [1] **Ross N.L.** (1987) High-pressure phase transitions in minerals. In: McGraw-Hill Encyclopedia of Science and Technology, McGraw-Hill, New York.
- [2] **Ross N.L.**, Angel R.J., Finger L.W., Hazen R.M., and Prewitt C.T. (1987) Oxygen-defect perovskites and the 93 K superconductor. Chapter 16 in 'Chemistry of high-temperature superconductors', American Chemical Society Symposium Series, volume 354.
- [3] Price G.D., and **Ross N.L.**, eds (1992) The Stability of Minerals, Chapman & Hall, London, 368pp.
- [4] **Ross N.L.** and Price G.D. (1992) Factors controlling mineral stability. In: Stability of Minerals. G.D. Price, N.L. Ross (eds.)Chapman & Hall, pp. 1-24.
- [5] **Ross N.L.** (1992) Lattice vibrations and mineral stability. In: Stability of Minerals. G.D. Price, N.L. Ross (eds.) Chapman & Hall, pp. 132-171.
- [6] **Ross N.L.** and Sowerby J.R. (1996) Crystal field spectrum of synthetic clinoferrosilite. In: Mineral Spectroscopy: A Tribute to Roger G. Burns. M.D. Dyar, C. McCammon, W. Schaefer (eds.) The Geochemical Society, Special Publication No. 5, pp. 273-280.
- [7] **Ross, N.L.** (2000) Framework structures. In: Reviews in Mineralogy and Geochemistry Vol.41: High-Temperature and High-Pressure Crystal Chemistry, R.M. Hazen and R.T. Downs, Eds., pp. 257-287, Mineralogical Society of America, Washington D.C.
- [8] **Ross, N.L.** and Downs, R.T. (2004) Gigh-Pressure Crystal Chemistry: "Stuffed" framework structures at high pressure. In: NATO ASI Series: High-Pressure Crystallography, P.F. McMillan and A. Katrusiak, Eds., Kluwer Academic Press, 457-474.