

Virginia Tech Crystallography Laboratory



Publications 2004

<http://www.crystal.vt.edu/crystal/>

- [1] Angel, R.J. "Absorption corrections for diamond-anvil cells implemented in the software package Absorb 6.0." *Journal of Applied Crystallography*, **2004**, *37*, 486-492.
- [2] Angel, R.J. "Some practical aspects of studying equations of state and structural phase transitions at high pressure." In: Katrusiak A, McMillan P (Eds) High-Pressure Crystallography. Kluwer Academic Publishers, **2004**, pp 21-36.
- [3] Angel, R.J. "Equations of state of plagioclase feldspars," *Contributions to Mineralogy and Petrology*, **2004**, *146*, 506-512.
- [4] Angel, R.J.; Bismayer, U; Marshall, W.G. "Local and long range order in ferroelastic lead phosphate at high pressure," *Acta Crystallographica*, **2004**, *B60*, 1-9.
- [5] Deck, P. A.; Konate, M. M.; Kelly, B. V.; Slebodnick, C. "C-F Activation Reactions of (Pentafluorophenyl)cyclopentadiene 3-(Pentafluorophenyl)indene with Tetrakis(dimethyl-amido)titanium(IV)," *Organometallics*, **2004**, *23*, 1089-97.
- [6] Gibbs, G.V; Cox, D.F; Ross, N.L. "A modeling of favorable H-docking sites and defects in the high pressure silica polymorph stishovite." *Physics and Chemistry of Minerals*, **2004**, *31*, 232-239.
- [7] Huang, F. H.; Jones, J. W.; Slebodnick, C.; Gibson, H. W. "Ion pairing in fast-exchange host-guest systems: Concentration dependence of apparent association constants for complexes of neutral hosts and divalent guest salts with monovalent counterions," *J. Am. Chem. Soc.*, **2003**, *125*, 14458-64.
- [8] Huang, F. H.; Gibson, H. W.; Bryant, W. S.; Nagvekar, D. S.; Fronczek, F. R. "First Pseudorotaxane-Like [3]Complexes Based on Cryptands and Paraquat: Self Assembly and Crystal Structures," *J. Am. Chem. Soc.*, **2003**, *125*, 9367-71.
- [9] Huang, F.; Nagvekar, D. S.; Slebodnick, C.; Gibson, H. W.* "A Supramolecular Triarm Star Polymer from a Homotritopic Tris(Crown Ether) Host and a Complementary Monotopic Paraquat-Terminated Polystyrene Guest by a Supramolecular Coupling Method," *J. Am. Chem. Soc.* **2005**; *127*; 484-485.

- [10] Koch, M; Woodland, A.B; Angel, R.J. "Stability of spinelloid phases in the system Mg₂SiO₄–Fe₂SiO₄–Fe₃O₄ at 1100C and up to 10.5 GPa." *Physics of the Earth and Planetary Interiors*, **2004**, 143-144:178-183.
- [11] McCammon, C.A; Frost, D.J; Smyth, J.R; Lausten, H.M.S; Kawamoto, T; Ross N.L; and Van Aken, P.A; "Oxidation state of iron in hydrous mantle phases: Implications for subduction and mantle oxygen fugacity," *Physics of Earth and Planetary Interiors*, **2004**, 144: 157-169.
- [12] Ross, N.L; Zhao, J; Burt, J; Chaplin, T.D. "Equations of state of GdFeO₃ and GdAlO₃ perovskites", *J Phys: Condensed Matter*, **2004**, 16, 5721-5730.
- [13] Ross, N.L; Zhao J; Angel R.J. "High-pressure structural behavior of GdAlO₃ and GdFeO₃ perovskites", *Journal of Solid State Chemistry*, **2004**, 177, 3768-3775.
- [14] Ross, N.L; Zhao, J; Angel R.J. "High-pressure single-crystal X-ray diffraction study of YAlO₃ perovskite", *J Solid State Chem.*, **2004**, 177, 1276-1284.
- [15] Slebodnick, C.; Zhao J; Angel R.J.; Hanson, B.E; Song, Y; Liu, Z; Hemley, R.J. "A High Pressure Study of Ru₃(CO)₁₂ by X-ray Diffraction, Raman and Infrared Spectroscopy", **2004**, *Inorg. Chem.* 43, 5245-5252.
- [16] Speziale, S; Duffy T.S; Angel, R.J. "Single crystal elasticity of fayalite to 12 GPa" *Journal of Geophysical Research*, **2004**, doi: 10.1029/2004JB003162.
- [17] Wang, G.; Slebodnick, C.; Butcher, R. J.; Tam, M. C.; Crawford, T. D.; Yee, G. T. *; "A Family of Decamethylmetallocene Charge-Transfer Salt Magnets Using Methyl Tricyanoethylenecarboxylate (MTCE) as the Electron Acceptor," *J. Am. Chem. Soc.* **2004**, 126, 16890-5.
- [18] Zhao, J; Ross, N.L; Angel R.J. "Tilting and distortion of CaSnO₃ perovskite to 7 GPa determined from single-crystal X-ray diffraction", *Phys Chem Mineral.*, **2004**, 31, 299-305.
- [19] Zhao, J; Ross, N.L; Angel R.J. "New view to explain high-pressure behavior of GdFeO₃-type perovskites", *Acta Cryst.* **2004**, B60, 263-271.
- [20] Zhao, J; Ross, N.L; Angel R.J. "Polyhedral control of the rhombohedral to cubic phase transition in LaAlO₃ perovskite". *J. Phys: Condensed Matter*, **2004**, 16, 8763-8773.
- [21] Angel, R.J; Ross, N.L; Zhao, J. "The compression of framework mineral: beyond rigid polyhedra," *European Journal of Mineralogy*, Accepted.
- [22] Benusa, M.D; Angel, R.J.; Ross, N.L. "Compression of Albite, NaAlSi₃O₈," *American Mineralogist*, in press.
- [23] Burt, J.B; Ross, N.L; Angel, R.J; Koch, M. "Equations of State and Structures of Andalusite and Sillimanite to 10 GPa," *American Mineralogist*, submitted.
- [24] Crichton, W; Ross N.L; "Equations of State of Dense Hydrous Silicates: Results from Single-Crystal X-ray Diffraction," *Mineralogical Magazine*, in press.
- [25] Fan, J; Slebodnick, C; Angel, R.J; Hanson, B. E.* "New Zinc Phosphates Decorated by Imidazole-Containing Ligands." *Inorg. Chem.* ASAP article.

- [26] Gibbs, G.V; Cox, D.F; Ross, N.L; Crawford, T.D; Burt, J; Rosso, K.M. “A mapping of the electron localization function for earth materials: A study of bonded interactions and model lone- and bond-pair domains.” *Physics and Chemistry of Minerals*, in press.
- [27] Huang, F; Slebodnick, C; Ratliff, A.; Gibson, H. W. “A Bis(m-phenylene)-32-crown-10/Monopyridinium [2]Pseudorotaxane” *J. Am. Chem. Soc.*, submitted.
- [28] Huang, F; Slebodnick, C; Gibson, H. W. “Cryptand/Monopyridinium [2]Pseudorotaxanes” *Angew. Chem.* **2005**, submitted.
- [29] Huang, F.; Slebodnick, C.; Gibson, H. W. “[3]Pseudorotaxanes Based on the Cryptand/Monopyridinium Salt Recognition Motif,” *J. Chem. Soc. Chem. Comm.* **2005**, submitted.
- [30] Huang, F.; Switek, K. A.; Zakharov, L. N.; Fronczek, F. R.; Slebodnick, C.; Lam, M.; Golen, J. A.; Bryant, W. S.; Mason, P.; Rheingold, A. L.; Ashraf-Khorassani, M.; Gibson, H. W. “Cryptands, Powerful Hosts for Paraquat Derivatives” *J. Am. Chem. Soc.* , submitted.
- [31] Tyree, W. S.; Slebodnick, C.; Spencer, M. C.; Wang, G.; Merola, J. S.; Yee, G. T. *Polyhedron*, in press.
- [32] Van Aken, P; Miehe, G; Woodland, A.B; Angel, R.J. “Crystal Structure and Cation Distribution in Fe₇SiO₁₀ (“Iskorite”).” *European Journal of Mineralogy*, submitted.