

# Virginia Tech Crystallography Laboratory



## Publications 2005

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

- [1] Angel RJ (2005) High-pressure structure determination and refinement by X-ray diffraction. In J Chen, et al. (eds.), *Frontiers in High-Pressure Research*, Elsevier, vol. (Xcalibur-2)
- [2] Angel RJ, Ross NL, Zhao J (2005) The compression of framework minerals: beyond rigid polyhedra. *European Journal of Mineralogy* 17:193-199.
- [3] Angel RJ, Zhao J, Ross NL (2005) General rules for predicting phase transitions in perovskites due to octahedral tilting. *Physical Review Letters* 95:025503. (Xcalibur1, Huber)
- [4] Benusa M, Angel RJ, Ross NL (2005) Compression of albite, NaAlSi<sub>3</sub>O<sub>8</sub>. *American Mineralogist* 90:1115-1120. (Xcalibur-1, Huber)
- [5] Brown JM, Abramson EH, Angel RJ (2005) Triclinic elastic constants for low albite. *Physics and Chemistry of Minerals* submitted:(Huber)
- [6] Bujak M, Angel RJ (2005) Single crystal X-ray diffraction studies on [(CH<sub>3</sub>)<sub>n</sub>NH<sub>4-n</sub>]<sub>3</sub>[Sb<sub>2</sub>Cl<sub>9</sub>] (n = 2, 3) chloroantimonates(III) in their low-temperature ferroelectric phases - structures and phase transitions. *Journal of Solid State Chemistry* 178:2237-2246. (Xcalibur-2)
- [7] Bujak M, Angel RJ (2005) Temperature- and pressure-induced structural changes in [(CH<sub>3</sub>)<sub>2</sub>NH(CH<sub>2</sub>)<sub>2</sub>NH<sub>3</sub>][SbCl<sub>5</sub>] studied by the single-crystal diffraction method. *Journal of the American Chemical Society* submitted:(Xcalibur-1, Xcalibur-2, Huber)
- [8] Burt J, Gibbs GV, Cox DF, Ross NL (2005) ELF isosurface maps of the Al<sub>2</sub>SiO<sub>5</sub> polymorphs. *Physics and Chemistry of Minerals* in press.
- [9] Burt J, Ross NL, Angel RJ, Koch M (2005) Equations of State and Structures of Andalusite and Sillimanite to 10 GPa. *American Mineralogist* in press:(Xcalibur-1, Huber)
- [10] Crichton WA, Ross NL (2005) Equation of state of dense hydrous magnesium silicates: results from single-crystal X-ray diffraction. *Mineralogical Magazine* 69:273-287.
- [11] Fan J, Hanson BE (2005) A two-dimensional cationic lattice built from [Zn<sub>6</sub>(HPO<sub>4</sub>)<sub>2</sub>(PO<sub>4</sub>)]<sup>2+</sup> clusters. *Journal of the Chemical Society, Chemical*

- Communications* 2327-2329. (Xcalibur-2)
- [12] Fan J, Hanson BE (2005) Novel zinc phosphate topologies defined by organic ligands. *Inorganic Chemistry* 44:6998-7008. (Xcalibur-2)
- [13] Fan J, Slebodnick C, Angel RJ, Hanson BE (2005) New zinc phosphates decorated by imidazole-containing ligands. *Inorganic Chemistry* 44:552-558. (Xcalibur-2)
- [14] Fan J, Slebodnick C, Troya D, Angel RJ, Hanson BE (2005) Five new zinc phosphite structures: tertiary building blocks in the construction of hybrid materials. *Inorganic Chemistry* 44:2719-2727. (Xcalibur-2)
- [15] Gibbs GV, Cox DF, Ross NL, Crawford TD, Burt J, Rosso KM (2005) A mapping of the electron localization function for earth materials. *Physics and Chemistry of Minerals* 32:208-221.
- [16] Gibbs GV, Cox DF, Ross NL, Crawford TD, Downs RT, Burt JB (2005) Comparison of the electron localization function and deformation electron density maps for selected earth materials. *Journal of Physical Chemistry A* 109:10022-10027.
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- [19] Huang FH, Nagvekar DS, Slebodnick C, Gibson HW (2005) 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. *Journal of the American Chemical Society* 127:484-485. (Xcalibur-2)
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