Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Geometric simulation of structures containing rigid units STEPHEN WELLS, ASU — Much insight into the behaviour of the framework silicates can be obtained from the Rigid Unit model. I review results from geometric analyses [1] of framework structures, quantifying the significance of rigid unit motion in thermal disorder and in defect accomodation, and from a method of simulation [2,3] based on a whole-body 'geometric potential' rather than on interatomic potentials. I show the application of the geometric potential to the symmetry-constrained generation of hypothetical zeolite frameworks [4], and to the rapid generation of protein conformations using insights from rigid cluster decomposition [5]. 1. Wells, Dove and Tucker, Journal of Applied Crystallography, 37:536–544 (2004). 2. G.D. Gatta and S.A. Wells, Phys. Chem. Min. 31:1–10 (2004). 3. A. Sartbaeva, S. A. Wells, S. A. T. Redfern, J. Phys.: Condens. Matter 16, 8173 (2004) 4. M. M. J. Treacy, I. Rivin, E. Balkovsky, K. H. Randall and M. D. Foster, Micropor. Mesopor. Mater. 74, 121-132 (2004). 5. M.F. Thorpe, Ming Lei, A.J. Rader, Donald J. Jacobs, and Leslie A. Kuhn, Journal of Molecular Graphics and Modelling 19, 1:60 - 69, (2001).

Stephen Wells
ASU

Date submitted: 02 Dec 2004 Electronic form version 1.4