

CONTENTS OF No. 397, DECEMBER 1995

	<i>page</i>
S. A. T. REDFERN: Advances in computer modelling of mineral properties	585
B. WINKLER, V. MILMAN and M. C. PAYNE: <i>Ab initio</i> total energy studies of minerals using density functional theory and the local density approximation	589
L. VOČADLO, A. PATEL and G. D. PRICE: Molecular dynamics: some recent developments in classical and quantum mechanical simulation of minerals	597
A. L. ROHL and D. H. GAY: Modelling the morphology of minerals by computer	607
R. A. JACKSON, P. A. MEENAN, G. D. PRICE, K. J. ROBERTS, G. B. TELFER and P. J. WILDE: Deriving empirical potentials for molecular ionic materials	617
I. TSATSKIS and E. K. H. SALJE: Computer simulation of a microstructure in a potassium feldspar	623
M. T. DOVE, V. HEINE and K. D. HAMMONDS: Rigid unit modes in framework silicates	629
 <i>Petrology</i>	
B. SCHULZ, C. TRIBOULET and C. AUDREN: Microstructures and mineral chemistry in amphibolites from the wester Tauern Window (Eastern Alps), and <i>P-T</i> deformation paths of the Alpine greenschist–amphibolite facies metamorphism	641
M. D. KAMPATA, J. MOREAU, J. HERTOGEN, D. DEMAÏFFE, E. CONDLIFFE and N. F. MUYEMBA: Megacrysts and ultramafic xenoliths from Kundelungu kimberlites (Shaba, Zaire)	661
 <i>Experimental Mineralogy</i>	
A. R. LENNIE, S. A. T. REDFERN, P. F. SCHOFIELD and D. J. VAUGHAN: Synthesis and Rietveld crystal structure refinement of mackinawite, tetragonal FeS	677
E. MAKOVICKY and S. KARUP-MØLLER: The system Pd–Fe–Ni–S at 900 and 725°C	685
 <i>Mineralogy</i>	
J. GUTZMER, N. J. BEUKES, A. S. E. KLEYENSTUBER and A. M. BURGER: Magnetic hausmannite from hydrothermally altered manganese ore in the Palaeoproterozoic Kalahari manganese deposit, Transvaal Supergroup, South Africa	703
E.-A. PERSEIL and D. C. SMITH: Sb-rich titanite in the manganese concentrations at St. Marcel-Praborna, Aosta Valley, Italy: petrography and crystal-chemistry	717
G. R. WATT: High-thorium monazite-(Ce) formed during disequilibrium melting of metapelites under granulite-facies conditions	735
 <i>Short Communications</i>	
N. J. ELTON and J. J. HOOPER: Widenmannite from Cornwall, England: the second world occurrence	745
M. ARSLAN and B.E. LEAKE: High-Ti biotite bearing ignimbrites from the Zilan Valley near Ercis, Lake Van, Eastern Turkey	750
K. M. MACKENZIE, K. A. RODGERS and P. R. L. BROWNE: Tamarugite, NaAl(SO ₄) ₂ ·6H ₂ O, from Te Kopia, New Zealand	754
A. BOUDREAU: Formation of chlor- and fluor-apatite in layered intrusions: A comment	757
J. A. MANDARINO: New minerals recently approved by the Commission on New Minerals and Mineral Names, International Mineralogical Association	761
E. H. NICKEL: Definition of a mineral	767
New manuscript guidelines for the reporting of stable hydrogen, carbon, and oxygen isotope-ratio data	769
<i>Book Reviews</i>	771
Alphabetical Index	777
Book Reviews Index	786