

Author index

Almeida, R., H. Diez y Riega and D.A. Morales, On the Hellmann–Feynman theorem and the corrections to the energy in the Rayleigh–Schrödinger perturbation theory	28 (2000) 201
Amat, L., see Bach, A.	28 (2000) 59
Angulo, J.C., see Romera, E.	28 (2000) 341
Bach, A., L. Amat, E. Besalú, R. Carbó-Dorca and R. Ponec, Quantum chemistry, Sobolev spaces and SCF	28 (2000) 59
Balasubramanian, K., see Tan, H.	28 (2000) 213
Bán, M.I., see Stachó, L.L.	28 (2000) 241
Basu, S. and R.K. Roychoudhury, The coherent state and anharmonic oscillator description of nonlinear oscillation	28 (2000) 35
Berberan-Santos, M.N., see Pogliani, L.	28 (2000) 313
Besalú, E., see Bach, A.	28 (2000) 59
Bochicchio, R., L. Lain, A. Torre and R. Ponec, Topological population analysis from higher order densities. I. Hartree–Fock level	28 (2000) 83
Bollini, C.G., M. Giambiagi, M.S. de Giambiagi and A.P. de Figueiredo, Graphical linking of a MO multicenter bond index to VB structures	28 (2000) 71
Bungay, S.D., R.A. Poirier and R.J. Charron, Optimization of transition state structures using genetic algorithms	28 (2000) 389
Carbó-Dorca, R., see Bach, A.	28 (2000) 59
Charron, R.J., see Bungay, S.D.	28 (2000) 389
de Figueiredo, A.P., see Bollini, C.G.	28 (2000) 71
de Giambiagi, M.S., see Bollini, C.G.	28 (2000) 71
Dehesa, J.S., see Romera, E.	28 (2000) 341
Diez y Riega, H., see Almeida, R.	28 (2000) 201
Ding, S., see Yang, B.	28 (2000) 247
Ding, S., see Zheng, Y.	28 (2000) 193
Dömötör, G., see Stachó, L.L.	28 (2000) 241
Giambiagi, M., see Bollini, C.G.	28 (2000) 71
Gumel, A.B., W.F. Langford, E.H. Twizell and J. Wu, Numerical solutions for a coupled non-linear oscillator	28 (2000) 325
Han, K., see Yang, B.	28 (2000) 247
Hefferlin, R. and J. Knoll, On the use of Laplace's equation for global predictions of internuclear separation and dissociation energy	28 (2000) 169

Kliesch, W., Potential energy surface exploration with equilibrial paths.	
Part I: Theory	28 (2000) 91
Kliesch, W., Potential energy surface exploration with equilibrial paths.	
Part II: Application	28 (2000) 113
Knoll, J., see Hefferlin, R.	28 (2000) 169
Koga, T., see Romera, E.	28 (2000) 341
Lain, L., see Bochicchio, R.	28 (2000) 83
Langford, W.F., see Gumel, A.B.	28 (2000) 325
Liao, M., see Tan, H.	28 (2000) 213
Mercer, G.N., see Sidhu, H.S.	28 (2000) 353
Merkin, J.H., P.L. Simon and Z. Noszticzius, Analysis of the electrolyte diode. Electro-diffusion and chemical reaction within a hydrogel reactor	28 (2000) 43
Morales, D.A., see Almeida, R.	28 (2000) 201
Nelson, M.I., see Sidhu, H.S.	28 (2000) 353
Noszticzius, Z., see Merkin, J.H.	28 (2000) 43
Pogliani, L. and M.N. Berberan-Santos, Constantin Carathéodory and the axiomatic thermodynamics	28 (2000) 313
Poirier, R.A., see Bungay, S.D.	28 (2000) 389
Ponec, R., see Bach, A.	28 (2000) 59
Ponec, R., see Bochicchio, R.	28 (2000) 83
Romera, E., T. Koga, J.C. Angulo and J.S. Dehesa, Upper bounds to atomic electron densities in position and momentum spaces	28 (2000) 341
Roychoudhury, R.K., see Basu, S.	28 (2000) 35
Sidhu, H.S., M.I. Nelson, G.N. Mercer and R.O. Weber, Dynamical analysis of an elementary $X + Y \rightarrow P$ reaction in a continuously stirred tank reactor	28 (2000) 353
Simon, P.L., see Merkin, J.H.	28 (2000) 43
Smeyers, Y.G. and M. Villa, A study of the internal dynamics of trimethylamine by means of the non-rigid group theory	28 (2000) 377
Stachó, L.L., G. Dömötör and M.I. Bán, On the reaction path concept of Olender and Elber	28 (2000) 241
Szalkai, I., A new general algorithmic method in reaction syntheses using linear algebra	28 (2000) 1
Tan, H., M. Liao, Y. Wang, G. Wu and K. Balasubramanian, A flexible correlation group table (CGT) method for the relativistic configuration interaction wavefunctions	28 (2000) 213
Torre, A., see Bochicchio, R.	28 (2000) 83
Twizell, E.H., see Gumel, A.B.	28 (2000) 325
Vibók, Á., Generalization of the Hylleraas functional for calculating BSSE-free intermolecular interactions: further considerations	28 (2000) 207
Villa, M., see Smeyers, Y.G.	28 (2000) 377

Wang, Y., see Tan, H.	28 (2000) 213
Weber, R.O., see Sidhu, H.S.	28 (2000) 353
Wu, G., see Tan, H.	28 (2000) 213
Wu, J., see Gumel, A.B.	28 (2000) 325
Yang, B., K. Han and S. Ding, Application of dynamical Lie algebraic method to atom–diatomic molecule scattering	28 (2000) 247
Zheng, Y. and S. Ding, Potential energy surface for linear triatomic molecules: An algebraic method	28 (2000) 193
Živković, T.P., Vibrational isotope effect by the low rank perturbation method	28 (2000) 267
Živković, T.P., Vibrational isotope effect of linear and planar molecules: Deuterated bromoethenes	28 (2000) 287
Znojil, M., Perturbation method with triangular propagators and anharmonicities of intermediate strength	28 (2000) 139