

## Contents

### Theme issue: Modern theoretical chemistry

	Article ID		Article ID
<b>INTRODUCTION</b>			
Modern theoretical chemistry: the legacy of Prof. John N. Murrell AJ Stace and DC Clary	20170460	Hartree–Fock implementation using a Laguerre-based wave function for the ground state and correlation energies of two-electron atoms AW King, AL Baskerville and H Cox	20170153
<b>ARTICLES</b>			
Kinetics and dynamics of near-resonant vibrational energy transfer in gas ensembles of atmospheric interest AJ McCaffery	20170150	Isomers and energy landscapes of micro-hydrated sulfite and chlorate clusters JC Hey, EJ Doyle, Y Chen and RL Johnston	20170154
Statistical mechanics of binary mixture adsorption in metal–organic frameworks in the osmotic ensemble LJ Dunne and G Manos	20170151	Hamiltonian flow over saddles for exploring molecular phase space structures SC Farantos	20170148
Interactions of $C^+(^2P_1)$ with rare gas atoms: incipient chemical interactions, potentials and transport coefficients WD Tuttle, RL Thorington, LA Viehland, WH Breckenridge and TG Wright	20170156	Accessing the molecular frame through strong-field alignment of distributions of gas phase molecules KL Reid	20170158
$C_n$ ( $n = 2 - 4$ ): current status AJC Varandas and CMR Rocha	20170145	High-accuracy water potential energy surface for the calculation of infrared spectra II Mizus, AA Kyuberis, NF Zobov, VYu Makhnev, OL Polyansky and J Tennyson	20170149
Application of one-dimensional semiclassical transition state theory to the $CH_3OH + H \rightleftharpoons CH_2OH/CH_3O + H_2$ reactions X Shan and DC Clary	20170147	Dynamic simulations of many-body electrostatic self-assembly EB Lindgren, B Stamm, Y Maday, E Besley and AJ Stace	20170143
Quantum chemical study of the structure, spectroscopy and reactivity of $NO^+ \cdot (H_2O)_{n=1-5}$ clusters KA Linton, TG Wright and NA Besley	20170152	Probing the rate-determining region of the potential energy surface for a prototypical ion–molecule reaction C Xie, X Liu, BC Sweeny, TM Miller, SG Ard, NS Shuman, AA Viggiano and H Guo	20170146