
AUSTRALIAN JOURNAL OF
CHEMISTRY
AN INTERNATIONAL JOURNAL FOR CHEMICAL SCIENCE

Volume 71 Number 4 2018

CONTENTS

Foreword

Celebrating Professor Graham Chandler's 80th Birthday
A. Karton, G. Koutsantonis, M. Spackman **201**

Full Papers

First Year Introductory Chemistry at the University of Western Australia: Reflections and Perceptions
T. D. Clemons, R. B. Bucat, D. Spagnoli **203**

A Computational Investigation of the Uncatalysed and Water-Catalysed Acyl Rearrangements in Ingenol Esters
A. A. Kroeger, A. Karton **212**

Structure and Bonding in Hexa-tert-butyl-hexa-peri-hexabenzocoronene Sandwich Complexes of Ruthenium
M. Lein **222**

Investigating the Resonance in Nitric Acid and the Nitrate Anion Based on a Modern Bonding Analysis
M. Fugel, F. Kleemiss, L. A. Malaspina, R. Pal, P. R. Spackman, D. Jayatilaka, S. Grabowsky **227**

The S66 Non-Covalent Interactions Benchmark Reconsidered Using Explicitly Correlated Methods Near the Basis Set Limit
M. K. Kesharwani, A. Karton, N. Sylvetsky, J. M. L. Martin **238**

Beyond the Woodward-Hoffman Rules: What Controls Reactivity in Eliminative Aromatic Ring-Forming Reactions?
A. D. D. Wonanke, D. L. Crittenden **249**

Modelling the Effect of Conformation on Hydrogen-Atom Abstraction from Peptides
B. Chan, L. Radom **257**

Anion Photoelectron Spectroscopy and High Level *Ab Initio* Calculations of the Halide–Nitric Oxide Dimer Complexes
K. M. L. Lapere, A. J. McKinley, D. Wild **265**

Mechanism for Three-Component Ni-Catalyzed Carbonyl–Ene Reaction for CO₂ Transformation: What Practical Lessons Do We Learn from DFT Modelling?
B. Chan, Y. Luo, M. Kimura **272**

The Polymorphs of ROY: A Computational Study of Lattice Energies and Conformational Energy Differences
S. P. Thomas, M. A. Spackman **279**

Bromination of Acridine
G. S. Chandler, W. H. F. Sasse **285**

Facile Synthesis of Pentamethylcyclopentadienyl Ruthenium Half-Sandwich Complexes by Naphthalene Displacement
J. Stone, D. Jago, A. Sobolev, M. Spackman, G. Koutsantonis **289**

Is it Reasonable to Obtain Information on the Polarizability and Hyperpolarizability Only from the Electron Density?
D. Jayatilaka, K. K. Jha, P. Munshi **295**

Communications

A Safe and Simple Synthesis of 1,4-Bis(trimethylsilyl) buta-1,3-diyne
S. Bock, P. J. Low **307**

A Theoretical Study of the Astrochemical ¹³C¹²CS + H → ¹²C¹³CS + H Reaction
D. Talbi **311**