A General Discussion on Chemical Concepts from Quantum Mechanics was held at the University of Manchester, UK on 4th, 5th and 6th September 2006.

CONTENTS

INTRODUCTORY LECTURE

13 Spiers Memorial Lecture
Quantum chemistry: The first seventy years
Roy McWeeny

PAPERS AND DISCUSSIONS

31 Anatomy of bond formation. Bond length dependence of the extent of electron sharing in chemical bonds from the analysis of domain-averaged Fermi holes
Robert Ponec and David L. Cooper

43 Bonding indicators from electron pair density functionals
Miroslav Kohout

55 Source function description of metal–metal bonding in d-block organometallic compounds
Carlo Gatti and Davide Lasi
79 Forces in molecules
Jesús Hernández-Trujillo, Fernando Cortés-Guzmán, De-Chai Fang and
Richard F. W. Bader

97 On the definition of local spin in relativistic and nonrelativistic quantum chemistry
Markus Reiher

125 General Discussion

151 Calculation of negative electron affinity and aqueous anion hardness using Kohn–Sham
HOMO and LUMO energies
Frank De Proft, Nick Sablon, David J. Tozer and Paul Geerlings

161 The physical basis of the hard/soft acid/base principle
Paul W. Ayers

191 Use of DFT-based reactivity descriptors for rationalizing radical addition reactions: applicability and difficulties
Asit K. Chandra and Minh Tho Nguyen

203 Carboranes: chemical concepts derived from the AIM study of the experimental and
theoretical electron density distribution functions

217 On the accurate estimation of intermolecular interactions and charge transfer: the case of
TTF-CA
Pilar Garcia, Slimane Dahaoui, Claudine Katan, Mohamed Souhassou and
Claude Lecomte

237 General Discussion

261 The physical origin of large covalent–ionic resonance energies in some two-electron bonds
Philippe C. Hiberty, Romain Ramozzi, Lingchun Song, Wei Wu and Sason Shaik

273 Quantifying resonance through a Lewis Valence Bond approach: application to haloallyl
and carbonyl cations
Mathieu Linares, Stéphane Humbel and Benoit Braïda

285 The unusual electronic mechanism of the [1,5] hydrogen shift in (Z)-1,3-pentadiene predicted
by modern valence bond theory
Peter B. Karadakov, J. Grant Hill and David L. Cooper

299 On the interpretation of valence bond wavefunctions
Remco W. A. Havenith, Joop H. van Lenthe, Leonardus W. Jenneskens and
Jeroen J. Engelberts

309 Current-density maps as probes of aromaticity: Global and Clar π ring currents in totally
resonant polycyclic aromatic hydrocarbons
Erich Steiner, Patrick W. Fowler, Alessandro Soncini and Leonardus W. Jenneskens

325 Electron sharing indexes at the correlated level. Application to aromaticity calculations
Eduard Matito, Miquel Solà, Pedro Salvador and Miquel Duran

347 Critical analysis of the local aromaticity concept in polyaromatic hydrocarbons
Patrick Bultinck

367 General Discussion

403 Direct estimate of conjugation and aromaticity in cyclic compounds with the EDA method
Israel Fernández and Gernot Frenking

423 Charge transfer, chemical potentials, and the nature of functional groups: answers from
quantum chemical topology
A. Martín Pendás, E. Francisco and M. A. Blanco

439 Energy partitioning schemes: a dilemma
I. Mayer
Highly polar bonds and the meaning of covalency and ionicity—structure and bonding of alkali metal hydride oligomers
F. Matthias Bickelhaupt, Miquel Solà and Célia Fonseca Guerra

The dithiolene ligand—'innocent' or 'non-innocent'? A theoretical and experimental study of some cobalt–dithiolene complexes

General Discussion

CONCLUDING REMARKS

Concluding remarks
Brian T. Sutcliffe

ADDITIONAL INFORMATION

Poster titles
List of Participants
Index of Contributors