

EDITORIAL

Davor Margetić and Robert Vianello

Croat. Chem. Acta 82 (2009) CXVII

Scientific Journey of Zvonimir Maksić

Davor Margetić and Robert Vianello

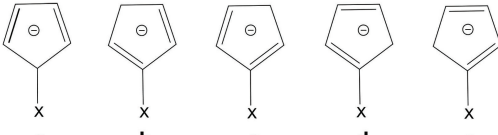
Croat. Chem. Acta 82 (2009) CXIX–CXXXI

ORIGINAL SCIENTIFIC PAPERS

CCA-3290

Acidity Enhancement of the Cyclopentadiene Ring by PH₂ and AsH₂ Substitution

Marcela Hurtado, Otilia Mó, Manuel Yáñez, and Jean-Claude Guillemin



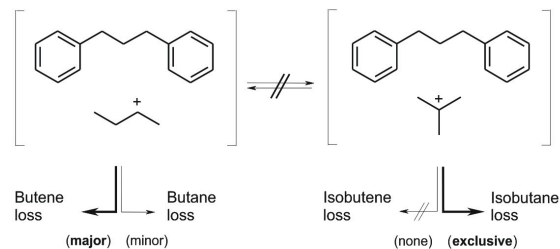
X = H	20	20	20	20	20
X = PH ₂	24.8	20.3	19.8	17.5	17.5
X = AsH ₂	24.3	20.1	19.8	17.9	17.8

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CCA-3291

Gaseous [C_nH_{2n+1}⁺ ... 1,3-Diphenylpropane] Ion/Neutral Complexes Containing Alkyl Cations of Different Acidities and Hydride Ion Affinities

Carsten Matthias and Dietmar Kuck

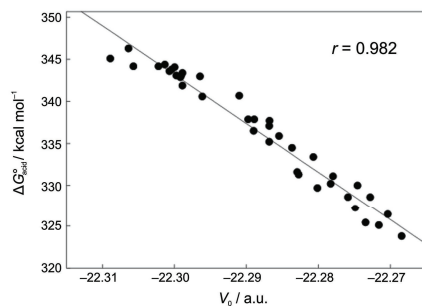


Croat. Chem. Acta 82 (2009) 7–19

CCA-3292

Predicting the Acidities of Substituted Phenols Using Electrostatic Potential at Nuclei

Maria Dimitrova and Boris Galabov

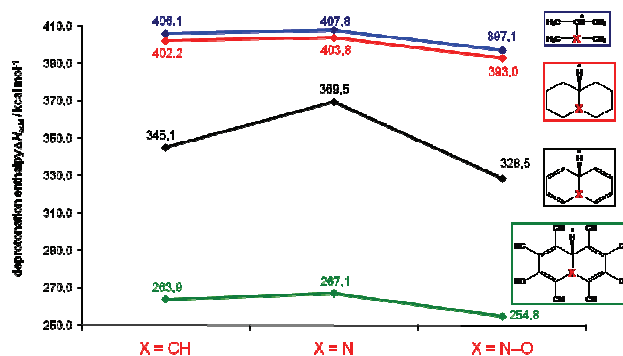


Croat. Chem. Acta 82 (2009) 21–25

CCA-3293

Acidifying Effect of an *N*-Oxide Group – A Useful Motif in Enhancing Acidity towards Supercritical Values

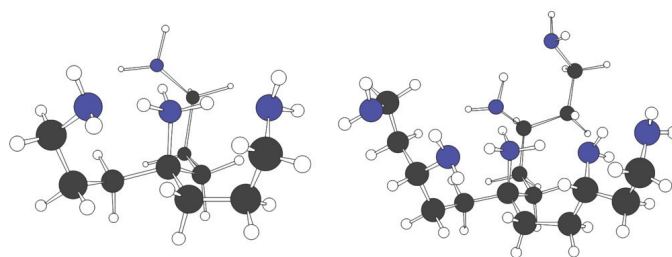
Robert Vianello

*Croat. Chem. Acta* **82** (2009) 27–39

CCA-3294

Neutral Intramolecular Hydrogen-bonded Bases

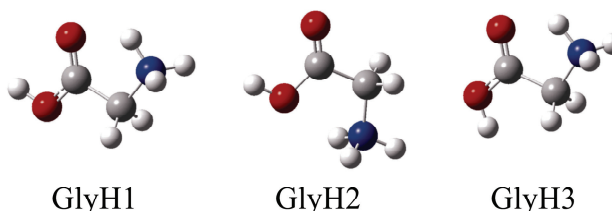
Zhixin Tian, Alireza Fattahi, Lev Lis, and Steven R. Kass

*Croat. Chem. Acta* **82** (2009) 41–45

CCA-3295

Gas-phase Basicity of Glycine

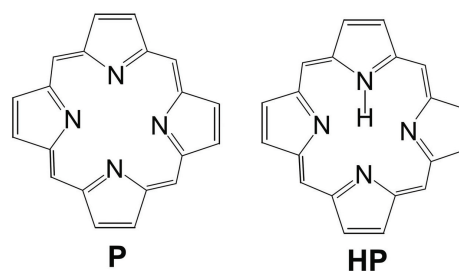
Guy Bouchoux and Ru Xuan Chia

*Croat. Chem. Acta* **82** (2009) 47–61

CCA-3296

Proton Affinities of Didehydroporphyrin and Subporphyrin in Ground and Excited States Obtained by Quantum Chemical Calculations

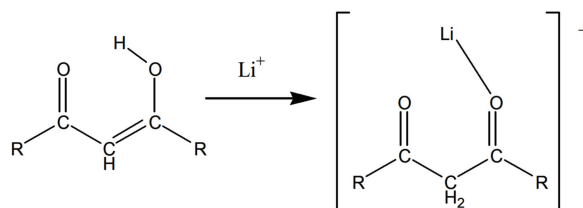
Zoran Glasovac, Mario Vazdar, and Davor Margetić

*Croat. Chem. Acta* **82** (2009) 63–70

CCA-3297

Proton and Lithium Cation Binding to Some β -Dicarbonyl Compounds. A Theoretical Study

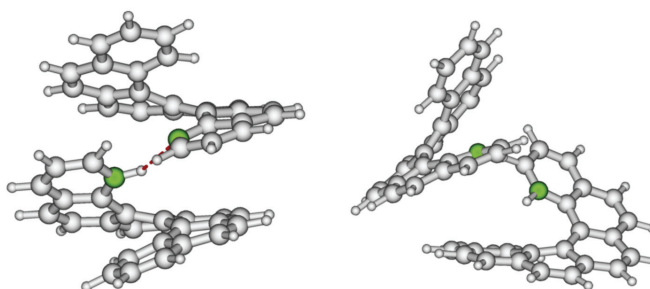
Peeter Burk, Kristo Taul, and Jaana Tammiku-Taul

*Croat. Chem. Acta* **82** (2009) 71–77*Croat. Chem. Acta* **82** (2009) CVII.

CCA-3298

Assembling Screws: Large Preference for the Homochiral Combination in the Proton-Bound Dimers of 1-Aza[6]helicene in the Gas Phase

Jiří Míšek, Miloš Tichý, Irena G. Stará, Ivo Starý, Jana Roithová, and Detlef Schröder

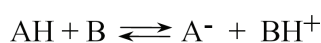


Croat. Chem. Acta **82** (2009) 79–86

CCA-3299

Proton Transfer Chemistry in the Gas Phase. Is a Spontaneous 'Neutralization' Reaction a Myth or a Reality?

Ewa D. Raczyńska, Jean-François Gal, Pierre-Charles Maria, and Małgorzata Szełąg



$$\delta_{\text{PT}}\Delta G^\circ = \text{GA}(\text{AH}) - \text{GA}(\text{BH}^+) =$$

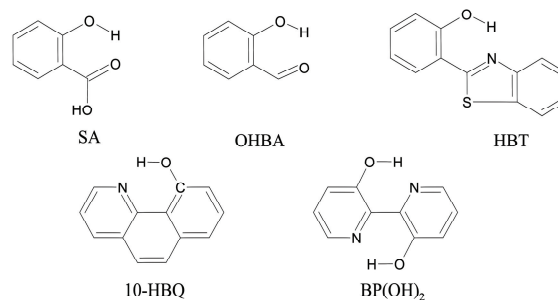
$$\text{GB}(\text{B}) - \text{GB}(\text{A}^-) < 0$$

Croat. Chem. Acta **82** (2009) 87–103

CCA-3300

Ultrafast Excited-state Proton Transfer Processes: Energy Surfaces and On-the-fly Dynamics Simulations

Adélia J. A. Aquino, Felix Plasser, Mario Barbatti, and Hans Lischka

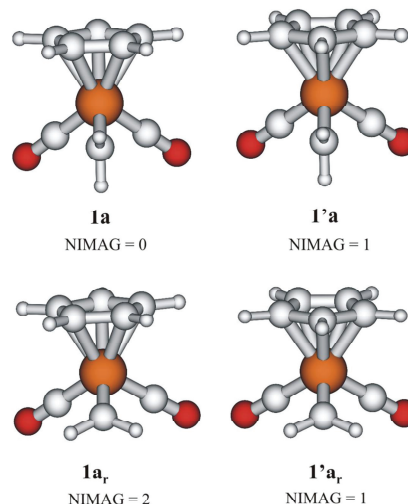


Croat. Chem. Acta **82** (2009) 105–114

CCA-3301

DFT Studies on Molecular and Electronic Structures of Cationic Carbene Complexes $[\text{L}_2(\eta^5\text{-C}_5\text{H}_5)\text{Fe}=\text{CR}_5]^+$ ($\text{L} = \text{CO}, \text{PH}_3, \text{dhpe}, \text{PPh}_3$; $\text{R} = \text{H}, \text{F}, \text{CH}_3$)

Isabella Hyla-Kryspin, Christian Mück-Lichtenfeld, and Stefan Grimme

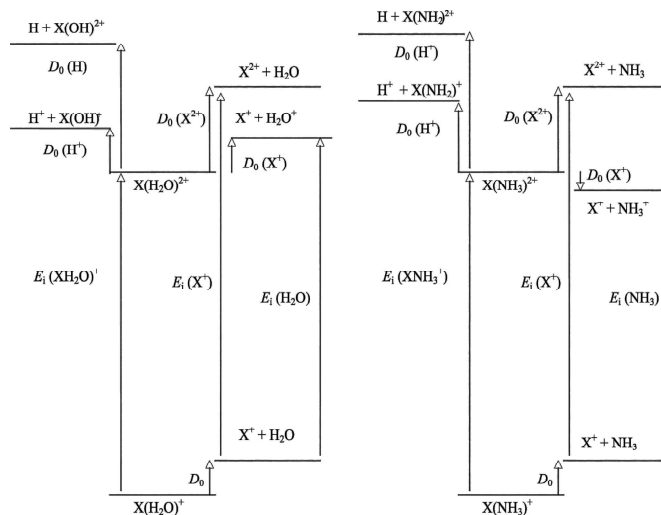


Croat. Chem. Acta **82** (2009) 115–127

CCA-3302

**Theoretical Study of Doubly Charged
[X(H₂O)] and [X(NH₃)] (X = Si, Ge, Sn, Pb)
Molecular Ions**

Pablo López-Tarifa, Fernando Martín,
Manuel Yáñez, and Manuel Alcamí

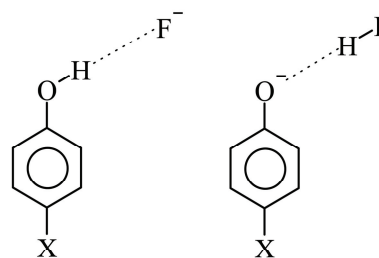


Croat. Chem. Acta **82** (2009) 129–137

CCA-3303

**Substituent Constants (σ_p^-) of the Rotated Nitro Group.
The Interplay Between the Substituent Effect of a Rotated
–NO₂ Group and H-Bonds Affecting π -Electron
Delocalization in 4-Nitrophenol and 4-Nitrophenolate
Complexes: a B3LYP/6-311+G** Study**

Michał A. Dobrowolski, Tadeusz M. Krygowski, and
Michał K. Cyrański



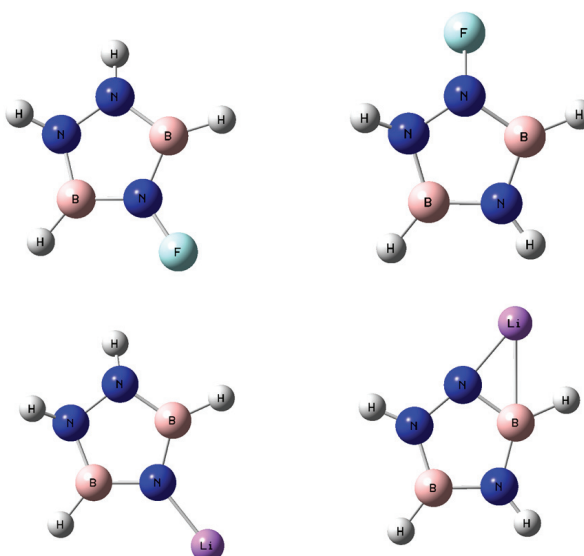
X = NO₂, H

Croat. Chem. Acta **82** (2009) 139–147

CCA-3304

**Substituent Effects on B–N Bonding and
Coupling Constants in Five-membered Rings
N₃B₂H₄X and N₂B₃H₄X, for X = H, F, and Li**

Janet E. Del Bene, Otilia Mó, and Manuel Yáñez



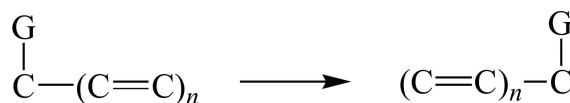
Croat. Chem. Acta **82** (2009) 149–155

Croat. Chem. Acta **82** (2009) CVII.

CCA-3305

Reformulating the Woodward-Hoffmann Rules in a Conceptual Density Functional Theory Context: the Case of Sigmatropic Reactions

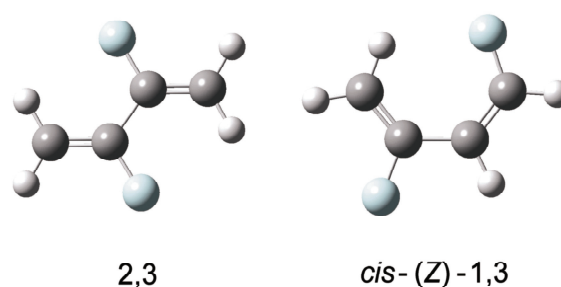
Nick Sablon, Frank de Proft, and Paul Geerlings

*Croat. Chem. Acta* **82** (2009) 157–164

CCA-3306

The Energetics of Halogenated Ethylenes (Ethyne)s and 1,3-Butadienes (Butadiynes): A Computational and Conceptual Study of Substituent Effects and “Dimerization”

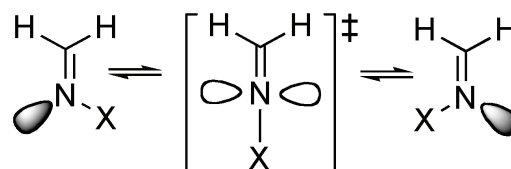
Carol A. Deakyne, Lawrence H. Warfel IV, Haunani M. Thomas, Dhananjaya Nauduri, Toyosi Esther A. Ajibowo, Nicole J. Carbonaro, Alec G. Simpson, and Joel F. Liebman

*Croat. Chem. Acta* **82** (2009) 165–172

CCA-3307

Barriers about Double Carbon-Nitrogen Bond in Imine Derivatives (Aldimines, Oximes, Hydrazones, Azines)

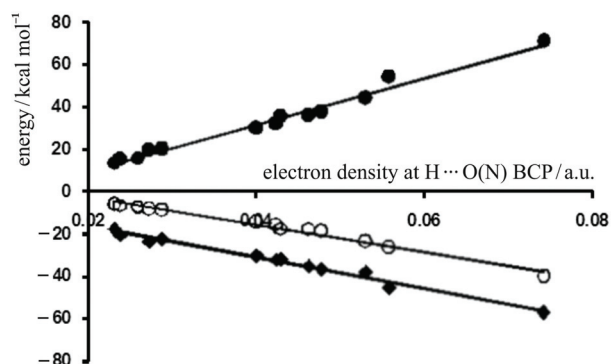
Fernando Blanco, Ibon Alkorta, and José Elguero

*Croat. Chem. Acta* **82** (2009) 173–183

CCA-3308

Covalent Character of Hydrogen Bonds Enhanced by π -Electron Delocalization

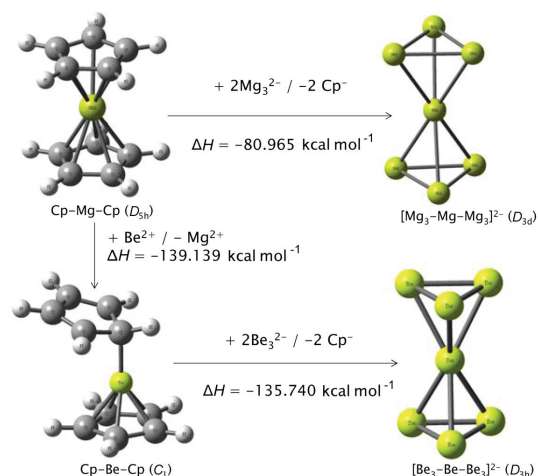
Sławomir Janusz Grabowski

*Croat. Chem. Acta* **82** (2009) 185–192

CCA-3309

Bonding, Reactivity and Aromaticity in Some Beryllocene Derivatives

Soma Duley, Puja Goyal, Santanab Giri, and Pratik Kumar Chattaraj

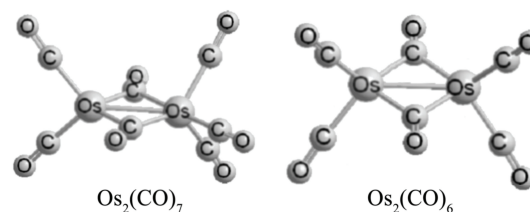


Croat. Chem. Acta **82** (2009) 193–205

CCA-3310

Heptacarbonyldiosmium and Hexacarbonyldiosmium: Two Highly Unsaturated Binuclear Osmium Carbonyls

Bing Xu, Qian-Shu Li, Yaoming Xie, Bruce King, and Henry F. Schaefer III

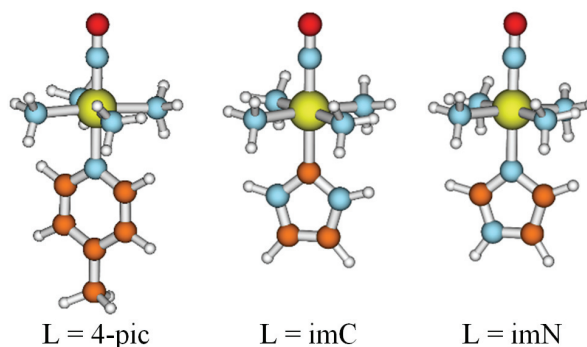


Croat. Chem. Acta **82** (2009) 207–218

CCA-3311

The Effects of N-Heterocyclic Ligands on the Nature of the Ru–(NO) Bond in Ruthenium Tetraammine Nitrosyl Complexes

Giovanni F. Caramori and Gernot Frenking

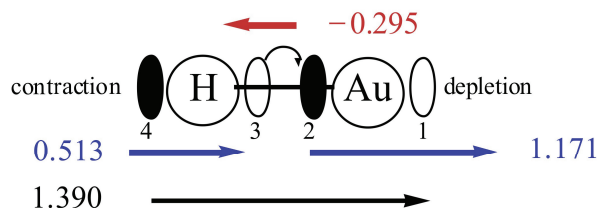


Croat. Chem. Acta **82** (2009) 219–232

CCA-3312

Comparison of Gold Bonding with Mercury Bonding

Elfi Kraka, Michael Filatov, and Dieter Cremer

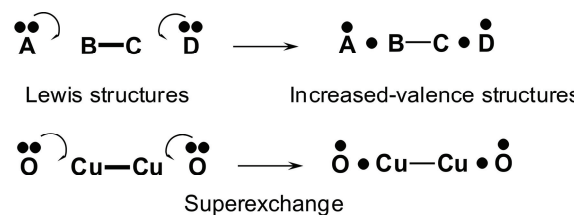


Croat. Chem. Acta **82** (2009) 233–243

CCA-3313

On the Magnetic Exchange Parameter for an O–Cu–Cu–O Component of Cu^{II} Carboxylate Dimers

Richard D. Harcourt

Croat. Chem. Acta **82** (2009) 245–251

CCA-3314

Dipole Polarizabilities of Fluorinated Hydrocarbons

Ladislav Éhn, Ivan Černušák, and Pavel Neogrady

Croat. Chem. Acta **82** (2009) 253–259

$$E(\mathbf{F}) = E^0 - \mu_a F_a - \frac{1}{2!} \alpha_{\alpha\beta} F_\alpha F_\beta - \dots$$

CCA-3315

On the Angular Independence of Sets of Atomic Orbitals

Joel F. Liebman and Zelek S. Herman

Croat. Chem. Acta **82** (2009) 261–265

$$S_n(\Theta) = N_0 + S_n(\Theta)$$

$$S_n(\Theta) = \sum_{j=1}^n \cos[(j-1) \cdot 2\pi\Theta]$$

CCA-3316

Molecular Surfaces, van der Waals Radii and Electrostatic Potentials in Relation to Noncovalent Interactions

Jane S. Murray and Peter Politzer

Croat. Chem. Acta **82** (2009) 267–275

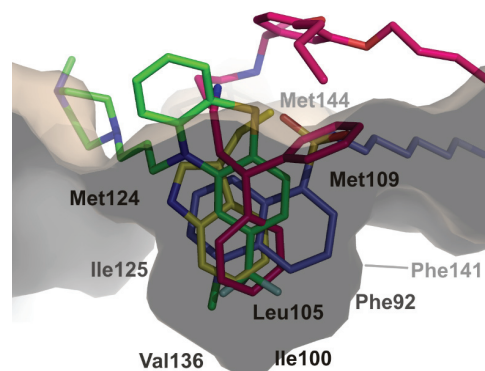
$$V(\mathbf{r}) = \sum_A \frac{Z_A}{|\mathbf{R}_A - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}') d\mathbf{r}'}{|\mathbf{r}' - \mathbf{r}|}$$

$$\nabla^2 V(\mathbf{r}) = 4\pi\rho(\mathbf{r}) - 4\pi \sum_A Z_A \delta(\mathbf{r} - \mathbf{R}_A)$$

CCA-3317

Theoretical Aspects of Molecular Recognition

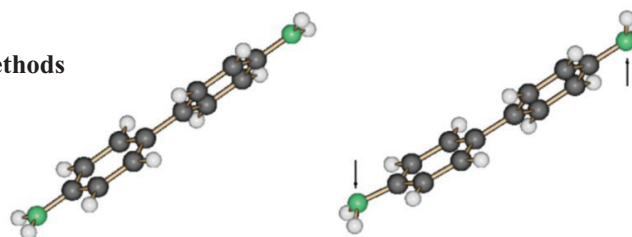
Veronika Harmat and Gábor Náray-Szabó

Croat. Chem. Acta **82** (2009) 277–282

CCA-3318

The Importance of Step Control in Optimization Methods

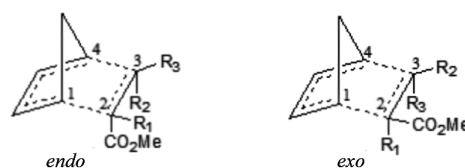
Jorge M. del Campo and Andreas M. Köster

Croat. Chem. Acta **82** (2009) 283–290

CCA-3319

Solvent Effects on the Stereoselectivity of Reaction of Methyl Acrylate, Methyl Methacrylate and Methyl *trans*-Crotonate with Cyclopentadiene: A Computational Study

Manoj K. Kesharwani and Bishwajit Ganguly

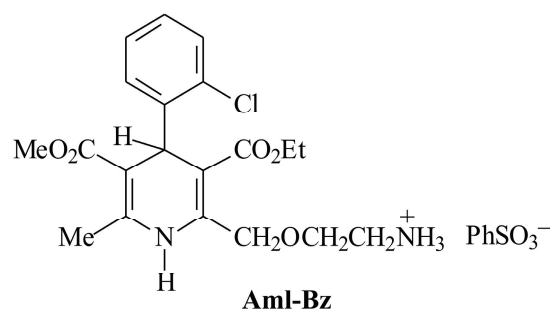
Croat. Chem. Acta **82** (2009) 291–298

$R_1 = R_2 = R_3 = H$ Cyclopentadiene + methyl acrylate
 $R_1 = CH_3, R_2 = R_3 = H$ Cyclopentadiene + methyl methacrylate
 $R_1 = R_2 = H, R_3 = CH_3$ Cyclopentadiene + *s-cis*-methyl-*trans*-crotonate

CCA-3320

Amlodipine Benzenesulfonate: A Mechanistic Investigation of Its Industrial Preparation via Detritylation of *N*-tritylamlopidine and Related NMR Studies

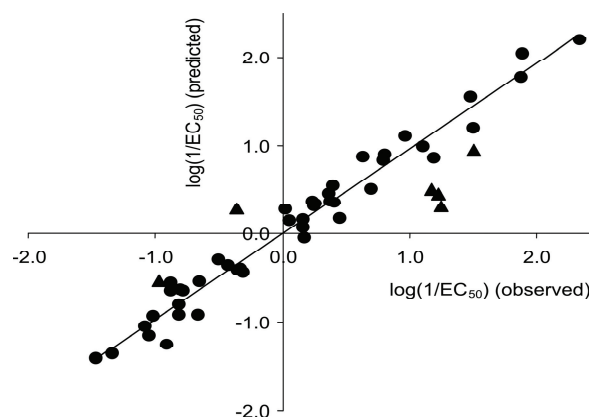
Borut Furlan, Simona Golič Grdadolnik, Stanko Hočevar, Darko Kocjan, Janez Levec, Howard Maskill, Hana Navrátilová, Jiří Pospíšil, Milan Potáček, Uroš Urleb, and Janko Žmitek

*Croat. Chem. Acta* **82** (2009) 299–309

CCA-3321

Predictions of Toxicity to *Chlorella vulgaris* and the Use of Momentum-space Descriptors

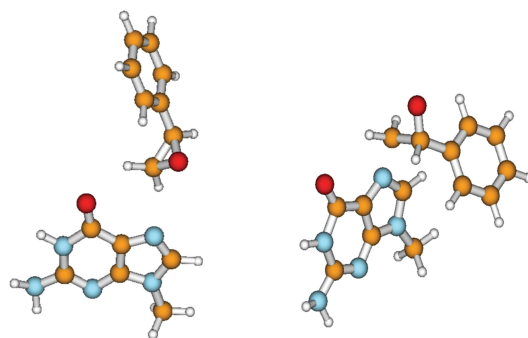
Jabir H. A. Al-Fahemi, David L. Cooper, and Neil L. Allan

Croat. Chem. Acta **82** (2009) 311–316*Croat. Chem. Acta* **82** (2009) CVII.

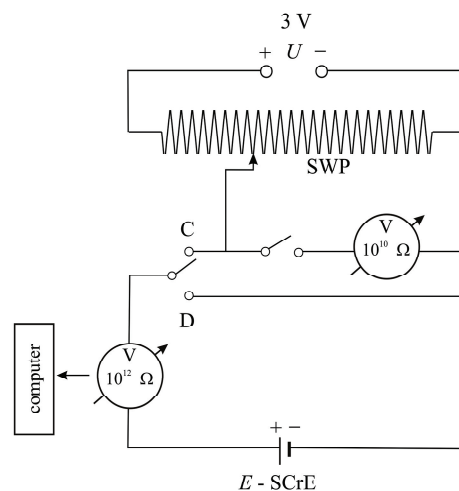
CCA-3322

**Carcinogenicity of Styrene Oxide:
Calculation of Chemical Reactivity**

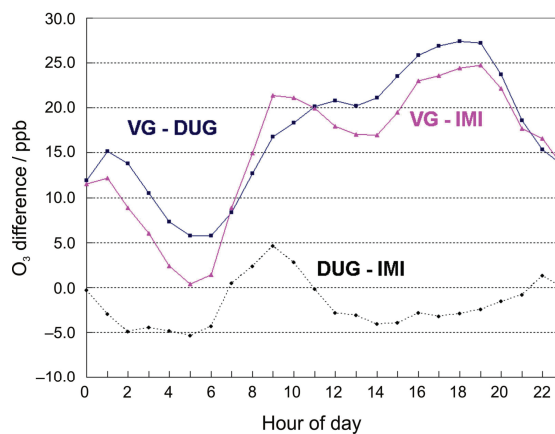
Mojca Kržan and Janez Mavri

*Croat. Chem. Acta* **82** (2009) 317–322

CCA-3323

**High Resistance Compensation Method for Surface
Potential Measurement**Nikola Kallay, Tajana Preočanin, Atiđa Selmani, Filip
Šupljika and Ivan Leniček*Croat. Chem. Acta* **82** (2009) 323–327

CCA-3324

Analysis of Summer 2006 Ozone Pollution in ZagrebGordana Pehnc, Leo Klasinc, Glenda Šorgo, and
Vladimira Vadić*Croat. Chem. Acta* **82** (2009) 329–335**APPENDIX****BOOK REVIEW**N. Trinajstić: Review of the book *Living Heritage of Vladimir Prelog*, by
M. Kaštelan-Macan

CXXXIII–CXXXIV

INSTRUCTIONS TO AUTHORS

CXXXV–CXXXIX

ANNOUNCEMENTS AND ADVERTISEMENTS

CXL–CXLII