



Society of Physical Chemists of Serbia

PHYSICAL CHEMISTRY 2021

*15th International Conference on
Fundamental and Applied Aspects of
Physical Chemistry*

PC2021

The Conference is dedicated to the

30th Anniversary of the founding of the Society of Physical Chemists of Serbia

and

100th Anniversary of Bray-Liebhafsky reaction



PHYSICAL CHEMISTRY 2021

15th International Conference on Fundamental and Applied Aspects of Physical Chemistry

Organized by

The Society of Physical Chemists of Serbia (SPCS)



in co-operation with

Institute of Catalysis, Bulgarian Academy of Sciences



Boreskov Institute of Catalysis, Siberian Branch of Russian Academy of Sciences



and

Members of the University of Belgrade:



Faculty of Physical Chemistry



Institute of Chemistry, Technology and Metallurgy



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and

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constructions of Ce-6-PWA and Ce-PWB were characterized by thermal analysis (TGA and DTA), X-ray powder diffraction (XRPD), and Fourier-transform infrared spectra (FTIR).

H-23-P

EVALUATION OF PERFORMANCE OF DISPERSION CORRECTED DENSITY FUNCTIONALS FOR TTF-TTF STACKING INTERACTIONS

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CCSD(T)/CBS energies for stacking interactions between two tetrathiafulvalene molecules were used as benchmark data to evaluate the performance of dispersion corrected density functionals in calculating the interaction energies. The results showed that the best functional for TTF-TTF stacking is B2PLYP-D3 with 6-311++G** basis set, which successfully reproduces gold standard CCSD(T)/CBS interaction energies. M06L-D3 functional with 6-311++G** basis set consistently underestimates interaction energies, giving potential energy curves of accurate shapes.

H-24-P

CHARACTERIZATION OF PRODUCTS OF PROLONGED HEMATOXYLIN AUTOXIDATION IN ALKALINE AQUEOUS SOLUTION

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The products of prolonged autoxidation of hematoxylin in alkaline aqueous solution were characterized by infrared (IR) spectroscopy, matrix-assisted laser desorption/ionization - time-of-flight mass spectrometry (MALDI-TOF MS), and electron spin resonance (ESR) spectroscopy. The IR data indicated that polymerization has occurred during this process. This was confirmed by the MALDI-TOF MS data, which also gave some insight into the degree of polymerization under our experimental conditions. The ESR data revealed that obtained products contain stable oxygen-centered radicals. This material has characteristics resembling natural and synthetic humic acid-like substances.