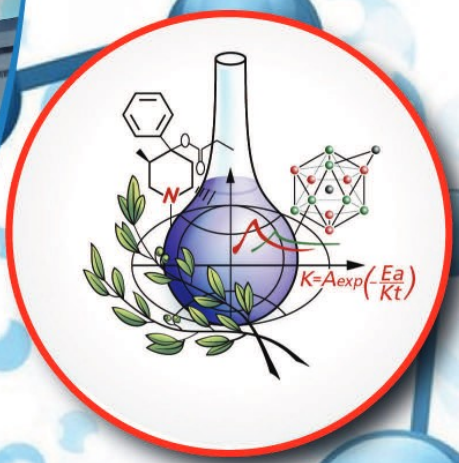
ADVANCES IN SYNTHESIS AND COMPLEXING



ADVANCES IN SYNTHESIS AND COMPLEXING

BOOK OF ABSTRACTS

The Sixth International Scientific Conference

Organic Chemistry
Inorganic and Coordination Chemistry
Physical and Colloidal Chemistry

26–30 September 2022
Moscow, RUDN University

Moscow
2022

MINISTRY OF SCIENCE AND HIGHER EDUCATION OF THE RUSSIAN FEDERATION
RUDN UNIVERSITY

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The book of abstracts of the Sixth International Scientific Conference: «Advances in Synthesis and Complexing» which was held from 26 to 30 September 2022 based on chemical departments of Faculty of Science of RUDN University includes abstracts of lectures of plenary, key-note and invited speakers, oral reports and poster session.

The present publication was designed to popularize scientific research activity in the field of chemistry and to discuss modern chemical problems on the international level. The digest is intended for scientists, students, postgraduates and for wide range of readers interested in problems in chemistry.

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Mixed isocyanide-phosphine complexes of palladium(II) dihalides

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Isocyanide ligands in platinum metal complexes exhibit strong σ-donor and weak π-acceptor properties, due to which such compounds are used as catalysts in important organic processes and in design of luminescent materials [1]. Of particular interest are mixed-ligand complexes containing, along with the isocyanide ligands, additional auxiliary neutral ligands, such as phosphines: appealing such approach, one can finely adapt the electronic and steric characteristics to target parameters [2, 3].

The complexes *cis*-[$PdCl_2$(CNR)(PPh_3)] (R = Mes **1**, Xyl **2**, ^{t}Bu **3**) were prepared by the bridge-splitting reaction of the dimer [$PdCl_2(PPh_3)]_2$ with corresponding isocyanides. The *cis*-[$PdBr_2$(CNR)(PPh_3)] (R = Mes **4**, Xyl **5**, ^{t}Bu **6**) were synthesized employing **1**–**3** and excess KBr in acetone at RT for ca. 4 d. These complexes are obtained as yellowish air- and moisture-stable solids and characterized by CHN elemental analyses, high-resolution mass spectrometry (ESI^+-HRMS), FT-IR, and ^{1}H, ^{31}P{^{1}H} and ^{13}C{^{1}H} NMR spectroscopy. The structures of **1** and **4**–**6** were established by single-crystal X-ray diffraction. All **1**–**6** are not subject to isomerization and are isomerically pure in the solid state and in $CDCl_3$ solution (*cis* configuration). The ligand metathesis reaction of **1**–**3** and KI in acetone at RT for approximately 3 h affords mixtures *cis/trans*-[PdI_2(CNR)(PPh_3)], *trans*-[PdI_2(CNR)$_2$)] and *trans*-[$PdI_2(PPh_3)_2$)].

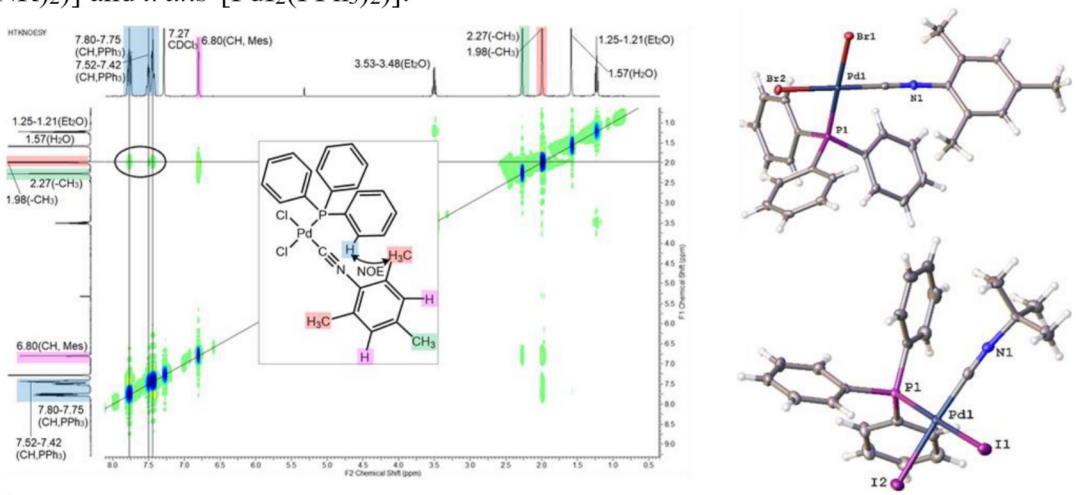

Fig. ^{1}H-^{1}H NOESY spectrum of **1** with indicated cross-peaks between protons of the CNMes and PPh_3 ligands (left) and X-ray molecular structures of **4** and *cis*-[PdI_2(CN^{t}Bu)(PPh_3)] (right).

This study was financially supported by the Russian Science Foundation (project no. 21-73-10083). Measurements were performed at the Center for Magnetic Resonance, Center for X-ray Diffraction Studies, Center for Chemical Analysis and Materials Research and Chemistry Educational Centre (all in St Petersburg University)

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