s13.m38.p7 Structural Study of Copper(II) Carboxylates with Some Derivatives of Pyridine. Marian Koman and Milan Melník, Department of Inorganic Chemistry, Faculty of Chemical and Food Technology, STU, Radlinského 9, 81237 Bratislava, Slovak Republic. E-mail: koman@chtf.stuba.sk

## Keywords: Copper; Carboxylates; Structure

The copper(II) carboxylates have been the subject of numerous investigations, especially with nitrogen donor ligands[1]. Copper(II) ions play a vital role in a number of widely differing biological processes, and their interaction with drugs administered for therapeutic reasons is of considerable interest. Some carboxylic acids and their derivatives also play an important role in biological processes[2-4]. Different coordination modes of of the carboxylato groups leads to the formation of mononuclear, binuclear and polynuclear structures. Over three hundred new $\mathrm{Cu}(\mathrm{II})$ coordination compounds with bioactive ligands were prepared in our laboratory. The crystal and molecular structures of 55 these new copper(II) coordination compounds with the composition of $\mathrm{CuX}_{2} \mathrm{~L}$ and $\mathrm{CuX}_{2} \mathrm{~L}_{2}(\mathrm{X}=$ fenamates, propionates and salicylates, as well as their derivatives) and $\mathrm{L}=$ nicotinamide, N,N-diethylnicotinamide, 2,6-dimethanolpyridine, 2-, 3- or 4-pyridincarbinol, were studied and classified. On the basis classification the evident trends of the structural type can by predict of the perspective new copper(II) compounds with familiar type of ligands. The X as well as some neutral ligands are active as non-steroidal antiphlogistic drugs. Therefore their study in the present of copper(II) is very promising.
[1] (a)Melník M.: Coord. Chem. Rev. (1981) 36, 287. (b)Kato M., Muto Y.: Coord. Chem Rev. (1988) 92, 45.
[2] Kozlevcar B., Lah N., Leban I. et al.: Croat. Chim. Acta (2000) 73, 733.
[3] Melník M., Koman M., Hudecová D. et al.: Inorg. Chim. Acta (2000) 308, 1.
[4] Koman M., Melnik M., Moncol J. et al.: Inorg. Chem. Comm. (2000) 3, 489.
s13.m38.p8 Synthesis and Crystal Structure of Ferrocene Derivatives. V. Kudar ${ }^{1}$, Gy. Túrós ${ }^{2}$, V. Zsoldos-Mády ${ }^{2}$, A. Csámpai ${ }^{I}$, M. Hanusz ${ }^{3}$, P. Sohár ${ }^{1,2}$, K. Simon ${ }^{3},{ }^{1}$ Dept. of Gen. and Inorg. Chem., ELTE, Budapest, ${ }^{2}$ Research Group for Structural Chemistry and Spectroscopy, Hung. Acad. Sci. - ELTE, Budapest, ${ }^{3}$ Chinoin Ltd, a member of Sanofi-Synthelabo Group, Budapest, Hungary. E-mail: zoldrepcsi@hotmail.com

Keywords: Ferrocene; X-ray single crystal analysis; Heterocyclic compounds

The study of ferrocene compounds has tremendously increased during the last two decades due to their applications in a variety of areas, including catalysis, organic synthesis and the design of new materials. There is rapidly growing interest in the use of transition-metal complexes in medicine and other biological areas as well.

We determined the crystal structure of six (1-6) ferrocene derivatives reported here.




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| Crystallographic parameters |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Compound | Space gruop | Unit cell |  | Volume/ $\AA^{3}$ | Z |
|  |  | $a / \AA, b / \AA, c / \AA$ | $\alpha /{ }^{\circ}, \beta /{ }^{\circ}, \gamma^{\circ}$ |  |  |
| 1 | P 21/c | $\begin{gathered} \hline 10.540(2) \\ 7.839(1) \\ 19.200(1) \\ \hline \end{gathered}$ | $\begin{gathered} 90 \\ 90.82(1) \\ 90 \end{gathered}$ | 1587.7(4) | 4 |
| 2 | P 21/c | $\begin{gathered} 7.420(2) \\ 16.331(2) \\ 17.004(2) \\ \hline \end{gathered}$ | $\begin{gathered} 90 \\ 90.43(1) \\ 90 \\ \hline \end{gathered}$ | 2060.5(6) | 4 |
| 3 | P-1 | $\begin{gathered} 9.446(5) \\ 9.844(2) \\ 17.955(8) \\ \hline \end{gathered}$ | $\begin{aligned} & 90.12(3) \\ & 98.09(5) \\ & 89.92(3) \\ & \hline \end{aligned}$ | 1652(1) | 2 |
| 4 | Pbca | $\begin{aligned} & 15.666(3) \\ & 10.853(3) \\ & 23.617(4) \\ & \hline \end{aligned}$ | $\begin{aligned} & 90 \\ & 90 \\ & 90 \\ & \hline \end{aligned}$ | 4015.4(7) | 8 |
| 5 | P 21/c | $\begin{gathered} 9.49(3) \\ 19.49(5) \\ 19.93(3) \\ \hline \end{gathered}$ | $\begin{gathered} 90 \\ 102.4(2) \\ 90 \end{gathered}$ | 3413(15) | 4 |
| 6 | P 21/c | $\begin{aligned} & 10.833(1) \\ & 10.425(2) \\ & 18.458(3) \end{aligned}$ | $\begin{gathered} 90 \\ 91.38(1) \\ 90 \end{gathered}$ | 2084.0(4) | 4 |

Structural features including the relative position of the two cyclopentadienyl rings will be discussed. Synthesis details of 3 [2] and 4-6 [1] are described elsewhere.
[1] A. Csámpai, Gy. Túrós, V. Kudar, K. Simon, H. Oeynhausen, H. Wamhoff and P. Sohár: Eur. J. Org. Chem. 4 (2004) 717-723.
[2] A. Csámpai, A. Abrán, V. Kudar, Gy. Túrós, H. Wamhoff and P. Sohár: Sythesis and structure determination of 1,1'-bis[pyridazin-3(2H)-one-6-yl]ferrocene and its ferrocenophane derivatives. Study on ferrocenes. Part 15.
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