m42.p08

New molecular conductors with cobalt bis(dicarbollide) anion

Olga Kazheva[a*], Anatolii Chekhlov[b], Vladimir Starodub[b], Oleg Dyachenko,[a]

[a]Department of Substance Structure, Institute of Problems of Chemical Physics, Chernogolovka, Russia. [b]Kharkov National University, Kharkov, Ukraine. E-mail: koh@icp.ac.ru

Keywords: structure-properties relationships, metallacarboranes, X-ray crystal structure analysis

At present only a few conducting radical cation salts containing metallacarborane anions were described [1-3]. It should be noted that no salts derived from the cobalt bis(dicarbollide) anion [3,3'-Co(1,2-$C_2B_9H_{11})_2]^-$, the most studied metallacarborane [4], were reported.
Here new electroconducting salts of cobalt bis(dicarbollide) anion: $(TMTSF)_2[Co(C_2B_9H_{11})_2]$ (**1**), $(TTF)[Co(C_2B_9H_{11})_2]$ (**2**) and $(ET)[Co(C_2B_9H_{11})_2]$ (**3**) were synthesized and investigated. The conductivity of crystals (**1**) at room temperature is 15 $Ohm^{-1}cm^{-1}$, which is the maximal value for metallacarborane salts. The comparison of the crystal structures of salts (**1**) and (**2**) showed, that the substitution of more prolate and volumetric TMTSF cation by a less prolate and volumetric TTF cation results in dramatic structural changes which allow us to explain the decrease of conductivity in (**2**) in comparison to (**1**) at 9 orders. Mainly it can be connected with the presence of conducting stacks of TMTSF cations in (**1**), while in (**2**) there are no stacks but pairs formed by TTF cations.
This work was supported by Russian Foundation for Basic Research (grants Nos. 04-03-97203, 05-03-32987).

[1] J.M. Forward, D.M.P. Mingos, et al., *J. Organomet. Chem*., 1994, 467, 207.
[2] Y.K. Yan, D.M.P. Mingos, et al.,*J. Chem. Soc., Chem. Comm*., 1995, 997.
[3] Y.K. Yan, D.M.P. Mingos, et al.,*J. Chem. Soc., Dalton Trans*., 1995, 3221.
[4] I.B. Sivaev, V.I. Bregadze, *Collect. Czech. Chem. Commun*., 1999, 64, 783.

m42.p09

Hydrogen Bonding and Structure-Activity Analysis of Some Antiandrogens

Olivera Klisurić,[a] Slobodanka Stanković,[a] Dušan Lazar,[a] Marija Sakač,[b] Kararina Penov-Gaši,[b] Evgenija Durendić,[b] Dieter Zobel[c], Armin Wagner[c]

[a]Department of Physics, University of Novi Sad, Serbia and Montenegro, [b]Department of Chemistry, University of Novi Sad, Serbia and Montenegro, and [c]Institute of Chemistry and Biochemistry-Crystallography, Freie University, Berlin, Germany. E-mail: olivia@uns.ns.ac.yu

Keywords: hydrogen bonding, steroids, X-ray diffraction

Androgen hormones, the group of steroid hormones, are mail sex hormones. They are vital to numerous physiological processes including development of mail sex organs and secondary mail sex characteristics. Beside their normal physiological functions, androgens can be responsible for growth and multiply of malignant cells, or can be cause of some other diseases (benign prostate gland hiperthense (BPH), prostate gland cancer, brain cancer, breast cancer, acnes, etc.). The fact that the androgens play the key role in many human diseases causes the intensive investigations in the field of obtaining and applying antiandrogens. Antiandrogens are substances which blockade the biological activities of androgens, and because of that they are used in therapy of some androgen-depend diseases. In our study of some androstene and adrostane derivatives with potentional antiandrogenic properties a number of androgenic compounds were synthesized, structurally analysed and tested for biologic effects. In this paper our attention was directed toward the examination of their hydrogen bonding characteristics. Examination of the structures of compounds having high affinity for androgen receptors led to the suggestion that steroid-receptor binding is primarily the result of interactions between the receptor and the steroidal D ring. Especially, of the great importance for the receptor binding are the position and the possible hydrogen bonds of H-atom from 17β-hydroxyl group. Activity of androgens might be controlled by the A ring and 3-oxo or 3-hydroxyl group. As a part of our study, the influences of molecule flexibility and substituents on the structure-activity relationship were also examined. The crystal structures of the compounds were determined by the single crystal X-ray diffraction methods. The energy minimum structures were obtained by molecular-mechanics calculations.

[1] Lazar D., Klisurić O., Stankoviac S., Penov-Gači K., Đurendić E., Kovačević R., Structure-activity relationships in 4- and 5-androstene: 3β-acetoxy-17-methyl-17-oxo-16,17-seco-5-androstene-16-carbonitrile and 17-methyl-3,17-dioxo-16,17-seco-4-androstene-16-carbonitrile, Acta Crystallographica Section C (2004). C60, 671 -673
[2] Duax W. L., Ghosh D., Pletnev V. and Griffin J. F., Three-dimensional structures of steroids and their protein targets, Pure & Appl. Chem., Vol. 68, No. 6, pp. 1297-1302, 1996.