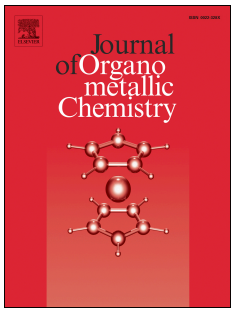
Accepted Manuscript



Synthesis and structure of Bis(Methylsulfanyl) derivatives of iron Bis(Dicarbollide)

Sergey A. Anufriev, Svetlana A. Erokhina, Kyrill Yu Suponitsky, Aleksei A. Anisimov, Julia N. Laskova, Ivan A. Godovikov, Fabrizia Fabrizi de Biani, Maddalena Corsini, Igor B. Sivaev, Vladimir I. Bregadze

PII: S0022-328X(18)30255-9

DOI: 10.1016/j.jorganchem.2018.04.019

Reference: JOM 20411

To appear in: *Journal of Organometallic Chemistry*

Received Date: 31 January 2018

Revised Date: 11 April 2018

Accepted Date: 12 April 2018

Please cite this article as: S.A. Anufriev, S.A. Erokhina, K.Y. Suponitsky, A.A. Anisimov, J.N. Laskova, I.A. Godovikov, F. Fabrizi de Biani, M. Corsini, I.B. Sivaev, V.I. Bregadze, Synthesis and structure of Bis(Methylsulfanyl) derivatives of iron Bis(Dicarbollide), *Journal of Organometallic Chemistry* (2018), doi: 10.1016/j.jorganchem.2018.04.019.

Synthesis and Structure of Bis(Methylsulfanyl) Derivatives of Iron Bis(Dicarbollide)[1]

Sergey A. Anufriev,[1] Svetlana A. Erokhina,[1] Kyrill Yu. Suponitsky,[1] Aleksei A. Anisimov,[2] Julia N. Laskova,[1] Ivan A. Godovikov,[1] Fabrizia Fabrizi de Biani,[3] Maddalena Corsini,[3] Igor B. Sivaev,[1] Vladimir I. Bregadze[1]

[1] *A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilov Str., 119991, Moscow, Russia*

[2] *D.I. Mendeleev Russian Chemical Technological University, 9 Miusskaya Sq., 125047, Moscow, Russia*

[3] *Dipartimento di Biotecnologie, Chimica e Farmacia, Università degli Studi di Siena, Via A. Moro 2, 53100 Siena, Italy*

Abstract. Bis(methylsulfanyl) derivatives of iron(II) bis(dicarbollide) [8,8′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2]^{2-}$ (**4**$^{2-}$), [4,4′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2]^{2-}$ (**5**$^{2-}$), and [4,7′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2]^{2-}$ (**6**$^{2-}$) were prepared by the treatment of the corresponding dimethylsulfonium derivatives **1**-**3** with potassium butylthiolate. Their oxidation by air in aqueous solution results in the corresponding derivatives of iron(III) bis(dicarbollide) [8,8′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2]^-$ (**7**$^-$), [4,4′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2]^-$ (**8**$^-$) and [4,7′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2]^-$ (**9**$^-$). The structures of $(Bu_4N)_2$[8,8′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2$] and (Me_4N)[4,7′-$(MeS)_2$-3,3′-Fe(1,2-$C_2B_9H_{10})_2$] were determined through single-crystal X-ray diffraction. In the solid state, the rotation of the dicarbollide ligands with respect to each other is hampered due to formation of weak intramolecular CH···S(Me) hydrogen bonds between the ligands resulting in stabilization of *transoid*-conformation in the case of 8,8′-isomer and *gauche*-conformation in the case of 4,4’-

[1] Dedicated to Professor Narayan Hosmane in recognition of his outstanding contribution in the field of carborane and metallacarborane chemistry and with very best wishes on the occasion of his 70th birthday.