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¹³C NMR and x-ray study of crystalline [Rh(Acac)(CO)₂] : no C_{2v} molecular symmetry in the solid state**Yuri Varshavsky, Tatiana Cherkasova, Margarita Galding, Alexander Korlyukov, Ivan Podkorytov, Vladimir Gindin, Sergey Smirnov, Anatoliy Rubaylo and Anton Mazur**

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¹³C NMR spectrum of [Rh (Acac) (CO)₂] (1) in solution (CDCl₃) contains four doublet signals (multiplicity/ chemical shift, ppm/ ¹³J, Hz/number of nuclei/group assignment): d/ 183.8/ 73.0/ 2C/ carbonyl ligands; d/ 187.4/ ~1/ 2C/ CO(Acac); d/ 101.8/ 2.6/ 1C/ CH; d/ 27.1/ 1.1/ 2C/ CH₃. ¹³C MAS NMR spectrum of the polycrystalline 1 displays 7 signals: d/ 185.4/ 70.7/1C and d/ 184.0/ 72.4/ 1C/ carbonyl ligands; s/ 188.1/1C and s/ 185.8/ 1C/ CO(Acac); s/ 100.3/ 1C/ CH; s/ 27.7/ 1C and s/ 27.0/ 1C/ CH₃. (They appear as 8 peaks). The results support our assumption based on the IR data that molecule 1 loses its C_{2v} symmetry on passing from the solution into the crystal. Inequivalence of carbonyl ligands in the molecule 1 may result from difference in their close surroundings in the crystal. For example, the contacts O...H-C of two CO ligands to methine group of the neighboring molecule in the adjacent stack (denoted with prime) are markedly different: (O)...(H)' 2.72 Å; (O)...(C)' 3.65 Å; angle(O)(H)'(C)' 164.9° for one CO ligand, and (O)...(H)' 4.38 Å; (O)...(C)' 5.00 Å; angle (O)(H)'(C)' 126.4° for the other.

Biography

Yuri Varshavsky earned his PhD degree in 1965 at the Kurnakov Institute of General and Inorganic Chemistry, Moscow, Russia. During the period 1967-1996, he was Head of laboratory at the Lebedev Institute of Synthetic Rubber, St. Petersburg, Russia. From 1997-2013, he worked as Head of Research Group at the Department of Chemistry at St. Petersburg State University. Having retired in 2014, he is currently involved, as an independent scholar, in the interpretation of experimental data obtained earlier by him and his colleagues. He has published more than 200 papers in peer-reviewed journals, delivered over 30 presentations at the international conferences, and received 10 patents. He also published (in co-authorship with M. I. Gelfman) a biography book about his scientific mentor, academician AA Grinberg. ("Nauka", Leningrad, 1974). His research interests are focused on the coordination chemistry of rhodium.

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