



Quadratic susceptibility and first hyperpolarizability of the complex of Cr(CO)(3) with 2.2 paracyclophane

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Auteur	Suponitsky, K. Y [1], Antonov, D. [2], Puntus, L. N [3], Smolyakov, A. F [4], Kajzar, François [5], Rau, Ileana [6], Sahraoui, Bouchta [7], Lyssenko, K. A [8]
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Résumé en anglais	The peculiarities of chemical bonding and nonlinear optical properties of the complex of Cr(CO)(3) with [2.2]paracyclophane (Cr-pCp) have been studied by a combined experimental-theoretical approach. The Cr-pCp complex exhibits second harmonic generation, the efficiency of which was measured by the powder technique at 1064.2 nm fundamental wavelength and estimated theoretically. The comparison of electronic structure of the Cr-pCp with benzene tricarbonyl chromium analogue has revealed an important role of intraligand charge transfer state in pCp moiety conditioned by a strong transannular interaction between aromatic rings which is responsible for the enhanced molecular hyperpolarizability of Cr-pCp.
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