

## Electronic structures of organometallic complexes of f elements. 62 [1] Parametric analysis of the crystal field splitting pattern of pseudo trigonal planar $\text{Nd}(\eta^5\text{-C}_5\text{Me}_4\text{H})_3$ .

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The absorption spectrum of pseudo ( $\Psi$ ) trigonal planar  $\text{Nd}(\eta^5\text{-C}_5\text{Me}_4\text{H})_3$  (**1**) has been measured at room and low temperatures. From the spectra obtained, a truncated crystal field (CF) splitting pattern could be derived, and simulated by fitting the parameters of a phenomenological Hamiltonian. For 38 assignments, a reduced r.m.s. deviation of  $30.7\text{ cm}^{-1}$  was achieved. On the basis of the CF parameters used, the global CF strength experienced by the  $\text{Nd}^{3+}$  central ion is estimated. The obtained Slater parameter  $F^2$  and the spin-orbit coupling parameter  $\xi_{4f}$  allow the insertion of compound **1** into truncated nephelauxetic and relativistic nephelauxetic series. Besides, the experimentally based non-relativistic molecular orbital scheme (in the f range) of complex **1** is set up and compared with the results of an SW- $X\alpha$  calculation on the fictive trigonal planar model complex  $\text{NdCp}_3$ .

### Adres publiczny

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