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Crystallographic report

Tris(η^5-cyclopentadienyl)-tetrahydrofuran-praseodymium

Peter C. Junk*

School of Chemistry, Monash University, Clayton, Vic. 3800, Australia

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The title compound is mononuclear with three η^5-cyclopentadienyl ligands and one tetrahydrofuran ligand. If the centroids of the cyclopentadienyl ligands are taken as the point of binding to praseodymium, then the environment about the metal centre is considered as a distorted tetrahedron.

KEYWORDS: praseodymium; cyclopentadienyl; crystal structure

COMMENT

$[Pr(Cp)_3(thf)]$ (Cp = η^5-cyclopentadienyl; thf = tetrahydrofuran) is a mononuclear compound and represents another member of the isomorphous $[Ln(Cp)_3(thf)]$ series for Ln = La,[1] Ce,[2] Nd,[3] Sm,[4] Gd,[5] Dy,[6] Er,[7] Yb,[8] Lu[9]). If the centroids of the Cp rings are considered as the site of binding to praseodymium, then the environment about the metal centre is a distorted tetrahedron (see Fig. 1 and caption for geometric parameters). The $Pr-Cp_{(centroid)}$ (average 2.54 Å) and Pr–O (2.551(2) Å) distances are intermediate between those of the adjacent Ln analogues in line with the variation in Ln^{3+} size.[10]

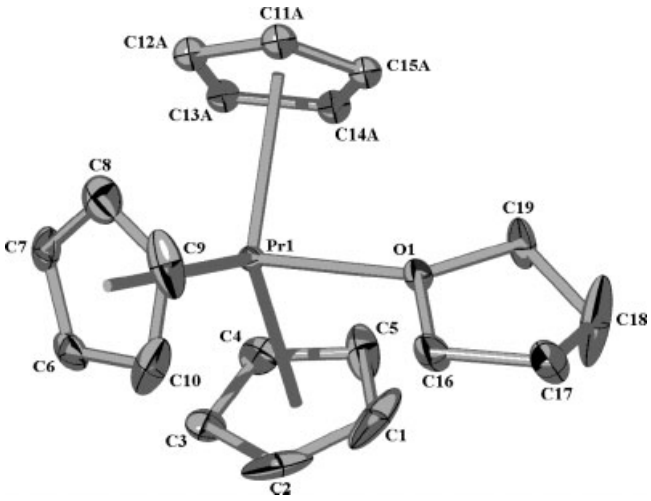

Figure 1. Molecular structure of $[Pr(Cp)_3(thf)]$. Important geometric parameters: Pr(1)–O(1) 2.551(2), Pr(1)–centroid(1) 2.52, Pr(1)–centroid(2) 2.54, Pr(1)–centroid(3) 2.55 Å; centroid(1)–Pr(1)–centroid(2) 119, centroid(1)–Pr(1)–centroid(3) 116, centroid(1)–Pr(1)–O(1) 96, centroid(2)–Pr(1)–centroid(3) 118, centroid(2)–Pr(1)–O(1) 101, centroid(3)–Pr(1)–O(1) 99°. Estimated standard deviations not given for centroids as these points are not refined.

EXPERIMENTAL

Synthesis

The literature procedure was followed.[11] Thus, to a solution of NaCp (0.20 mol) in thf, was added anhydrous $PrCl_3$ (9.81 g, 0.04 mol) and the solution stirred overnight, whereupon the solution was light green and a white precipitate settled. After filtration and concentration, light green crystals deposited after cooling at 0 °C. Yield: 90.6%.

Crystallography

Crystal data for: $C_{19}H_{23}OPr$, $M = 408.28$, $0.22 \times 0.30 \times 0.32$ mm^3, monoclinic, $P2_1/n$, $a = 8.253(3)$, $b = 24.380(8)$, $c = 8.370(3)$ Å, $\beta = 101.592(5)°$, $V = 1649.7(9)$ Å^3, $Z = 4$, $D_c = 1.644$ g cm^{-3}. Bruker SMART 1000 CCD diffractometer, $T = 223(2)$ K, $2\theta_{max} = 56.6°$, μ(Mo Kα) = 2.950 mm^{-1}, 10 527 reflections collected, 3926 unique, 3245 reflections with $I > 2\sigma(I)$. $R_1 = 0.028$ (obs. data), $wR_2 = 0.069$ (all data). The Cp ring (C11–C15) is disordered over two sites, but this was successfully modelled and there is high thermal motion in the thf molecule. Programs used: SAINT, SHELXL97, POVRAY, XSEED. CCDC number: 216999.

*Correspondence to: Peter C. Junk, School of Chemistry, Monash University, Clayton, Vic. 3800, Australia.
E-mail: peter.junk@sci.monash.edu.au

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