APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2005; **19**: 171–172
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.730

Crystallographic report

2,4-Diphenyl-1,3-bis(4,4,5,5-tetramethyl[1,3,2] dioxaborolan-2-yl)-buta-1*Z*,3*E*-diene

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Received 6 June 2004; Revised 14 June 2004; Accepted 15 June 2004

The compound comprises a 1*Z*,3*E*-butadiene moiety substituted by two pinacol boronate functional groups.

KEYWORDS: crystal structure; 1,3-butadiene; dioxaborolane

COMMENT

We have described the synthesis of a novel class of 1,3- and 1,4-diboryl-1,3-butadienes by zirconocene-mediated reductive cyclization of alkynylboronates followed by treatment with acid.[1] Although Metzler *et al*.[2] have prepared similar 1,4-diboryl-1,3-butadienes, a structural investigation of this class of compounds has not been reported. The molecular structure, Fig. 1, comprises a 1,3-butadiene moiety substituted by two pinacol boronate functional groups at C(13) and C(15), and a two phenyl groups at C(14) and C(16); bond distances and angles are typical.[3] The C14-phenyl and the C15-dioxaborolane groups are twisted out of the plane of the molecule, and the terminal groups are essentially planar. This arrangement is probably due to steric interactions between the dioxaborolane and phenyl groups. Since the B–O bond distances are similar to each other, we only included half the values.

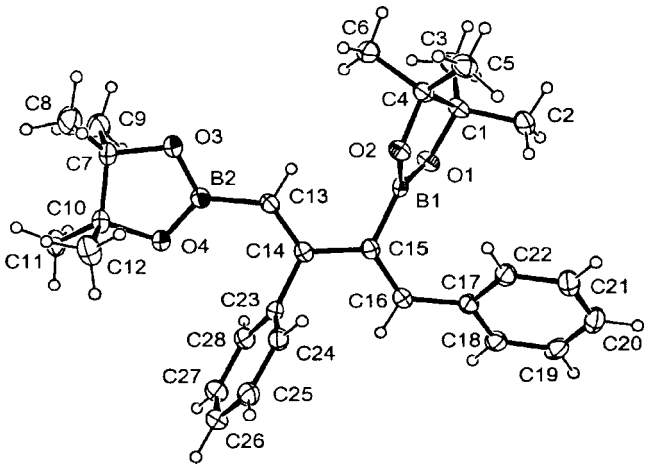

Figure 1. Molecular structure of $C_{28}H_{36}B_2O_4$. Selected bond distances and angles: B1–O2 1.370(2), B1–C15 1.578(3), B2–O4 1.371(2), B2–C13 1.552(3), C13–C14 1.350(3), C14–C15 1.488(2), C15–C16 1.350(3) Å; C13–C14–C15 121.71(17), C15–C14–C23 117.26(15), C14–C15–B1 118.04(16), C16–C15–B1 122.30(16)°.

EXPERIMENTAL

Colorless single crystals of the title compound suitable for X-ray diffraction analysis were obtained from a saturated pentane solution at −20 °C. Measurements were made at 110(1) K on a Nonius KappaCCD difractometer using Mo Kα radiation. Crystal data for: $C_{28}H_{36}B_2O_4$, $M = 458.19$, triclinic, space group $P\bar{1}$, $a = 6.0900(2)$, $b = 12.5500(7)$, $c = 17.0730(8)$ Å, $\alpha = 93.5230(19)$, $\beta = 90.074(3)$, $\gamma = 99.198(3)°$, $V = 1285.59$ Å^3, $Z = 2$, $R = 0.057$ (3899 reflections with $I \geq 2\sigma(I)$), $wR = 0.130$ (all 5978 reflections, $\theta_{max} = 28.2°$). Programs used: DENZO-SMN. Scalepack, SIR-97, SHELXL-97, ORTEP. CCDC deposition number: 240617.

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Contract/grant sponsor: Israeli Science Foundation; Contract/grant number: 138/01.
Contract/grant sponsor: Alex Grass Center for Drug Design and Synthesis of Novel Therapeutics.
Contract/grant sponsor: David R. Bloom Center of Pharmacy.

Acknowledgments

This research was supported by the Alex Grass Center for Drug Design and Synthesis of Novel Therapeutics, David R. Bloom Center of Pharmacy and the Israeli Science Foundation.

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