The structure of the title compound, [Cu(PPh₃)₂(BH₄)], has been redetermined at 90 K. The geometric parameters of the present structure agree with those previously studied at room temperature [Lippard & Melmed (1967). *Inorg. Chem.* 6, 2223–2228; Li *et al.* (2000). *Chin. J. Struct. Chem.* 19, 91–94], but with significantly improved precision. The molecule has twofold rotation symmetry.

**Comment**

The crystal structure of the title compound, (I), has been previously studied at room temperature (Lippard & Melmed, 1967; Li *et al.*, 2000). In the present redetermination, data were collected at low temperature, using a diffractometer equipped with a new APEX2 CCD area detector. As shown in Fig. 1, the structure of (I) is composed of neutral [Cu(PPh₃)₂(BH₄)] complex molecules with crystallographic twofold rotation symmetry. The results show that the coordination around Cuᴵ is distorted tetrahedral, with two triphenylphosphine P atoms [Cu–P₁ = 2.2780 (3) Å] and two H atoms of the bidentate tetrahydroborate anion [Cu–H₁B = 1.79 (2) Å], as in the pyridine solvate [Cu(PPh₃)₂(BH₄)]-pyridine (Engelhardt *et al.*, 1985). The geometric parameters of the present structure agree with those previously reported by Lippard & Melmed (1967) and Li *et al.* (2000), but with significantly improved precision. The precision of the Cu–P₁ bond length (0.0003 Å), the P–C bond lengths (mean 0.001 Å) and the C–C bond lengths (mean 0.0016 Å) for the low-temperature study are better than the room-temperature results reported by Lippard & Melmed (0.001, 0.005 and 0.008 Å, respectively) and Li *et al.* (0.001, 0.004 and 0.006 Å, respectively). Similarly, the standard uncertainty for the P₁–Cu–P₁ bond angle for the low-temperature data is 0.001°, whereas for both the room-temperature structures it is 0.006°.

**Experimental**

[Cu(PPh₃)₂(BH₄)] was prepared by a modification of the procedure reported by Fleet & Harding (1979). Finely powdered copper(I) chloride (0.40 g, 4 mmol) was added to a stirred solution of tri-
phenylphosphine (2.16 g, 8.2 mmol) in chloroform (10 ml) over a period of five minutes. The reaction mixture was stirred until the copper chloride had dissolved (30 min), treated with a solution of sodium tetrahydroborate (0.15 g, 4 mmol) in ethanol (3 ml), stirred for one hour, and then added to water (3 ml). The chloroform layer was then washed with water (3 ml), dried (magnesium sulfate) and filtrated. Crystals were grown by slowly diffusing diethyl ether vapor into a solution of \([\text{Cu}(\text{PPh}_3)_2(\text{BH}_4)]\) in chloroform.

**Crystal data**

\[\text{[CuP(C}_6\text{H}_5)_3}_2(\text{BH}_4)]\]

- \(M_r = 602.92\)
- Monoclinic, \(C 2/c\)
- \(a = 24.260 (1) \text{ Å}\)
- \(b = 9.0818 (5) \text{ Å}\)
- \(c = 15.0164 (8) \text{ Å}\)
- \(\beta = 115.516 (1) ^\circ\)
- \(V = 2985.8 (3) \text{ Å}^3\)
- \(Z = 4\)

**Data collection**

Bruker SMART APEX2
diffractometer
\(\omega\) scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
\(T_{\text{max}} = 0.813, T_{\text{min}} = 0.966\)
25 525 measured reflections
4344 independent reflections
with \(I > 2\sigma(I)\)

**Refinement**

Refinement on \(F^2\)

- \(R[F^2 > 2\sigma(F^2)] = 0.023\)
- \(wR(F^2) = 0.064\)
- \(S = 1.02\)
- 4344 reflections
- 190 parameters
- \(H\) atoms treated by a mixture of independent and constrained refinement

\(D_r = 1.341 \text{ Mg m}^{-3}\)

**References**


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