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Acetato[hydridotris(5-methyl-3-phenylpyrazol-1-yl-κN^2)borato]copper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.044
wR factor = 0.125
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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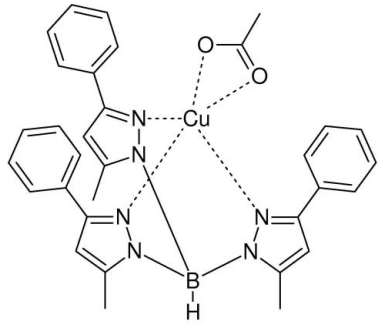
Reaction of potassium hydridotris(5-methyl-3-phenylpyrazoly)borate with copper(II) acetate in methanol at room temperature gives the title compound, $[Cu(C_{30}H_{28}BN_6)(C_2H_3O_2)]$. The Cu atom is five-coordinated by three N atoms from pyrazolyl groups and two O atoms from the acetate ligand.

Comment

The hydridotris(5-methyl-3-phenylpyrazoly)borate anion is one of the most important tripodal ligands for the design of model complexes of metalloenzymes (Parkin, 2004). Many crystal structures of zinc complexes of this ligand have been reported (Parkin, 2004), but only a few copper complexes have so far appeared in the literature (Chen *et al.*, 2000; Fujisawa *et al.*, 2000, 2001, 2004; Keij *et al.*, 1991; Kitajima *et al.*, 1990, 1992; Komiyama *et al.*, 2004; Sun *et al.*, 2003; Wada *et al.*, 2004). Structural analysis of copper complexes may help to elucidate the manner of interaction of the catalytic centers of metalloenzymes with various substrates/inhibitors. To this end, the title compound, (I), was prepared and characterized.



(I)

In (I), atom Cu1 is coordinated by three N atoms from pyrazolyl groups and two O atoms from the acetate anion (Table 1 and Fig. 1). The coordination geometry is distorted square pyramidal, with atom N6 in the apical position and atoms N1, N3, O1 and O2 forming the approximate square plane. The Cu1—N6 bond length is *ca* 0.3 Å longer than the average Cu—N1 and Cu—N3 bond lengths (Table 1).

Experimental

Equimolar quantities of potassium hydridotris(3,5-methylphenylpyrazoly)borate (Puert & Cohen, 2002) and copper(II) acetate (purchased from VWR) were separately dissolved in 10 ml methanol. The solutions were mixed and stirred for 30 min, and crystals were obtained by slow evaporation of the solution at room temperature.

Crystal data

$[Cu(C_{30}H_{28}BN_6)(C_2H_3O_2)]$
M_r = 605.98
Triclinic, $P\overline{1}$
a = 11.301 (18) Å
b = 12.035 (8) Å
c = 12.066 (15) Å
α = 112.97 (9)°
β = 97.09 (7)°
γ = 92.12 (10)°
V = 1493 (3) Å^3
Z = 2
D_x = 1.348 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 293 (2) K
Prism, green
0.10 × 0.10 × 0.10 mm

Data collection

Bruker 1000 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.924, T_{max} = 0.927
20842 measured reflections
5986 independent reflections
3916 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.01
5986 reflections
387 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.9974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.978 (4)	Cu1—N3	1.996 (3)
Cu1—O2	2.042 (4)	Cu1—N6	2.314 (4)
Cu1—N1	1.968 (4)		
N1—Cu1—O1	172.58 (10)	N3—Cu1—O2	149.51 (12)
N1—Cu1—N3	89.56 (14)	N1—Cu1—N6	86.19 (15)
O1—Cu1—N3	96.48 (14)	O1—Cu1—N6	97.22 (15)
N1—Cu1—O2	108.62 (14)	N3—Cu1—N6	97.71 (13)
O1—Cu1—O2	64.09 (14)	O2—Cu1—N6	107.48 (14)

Carbon-bound H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl groups. The methyl groups were allowed to rotate about their local threefold axes. Atom H1, bound to B1, was located in a difference Fourier map and refined freely with an isotropic displacement parameter [B—H = 1.16 (3) Å].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

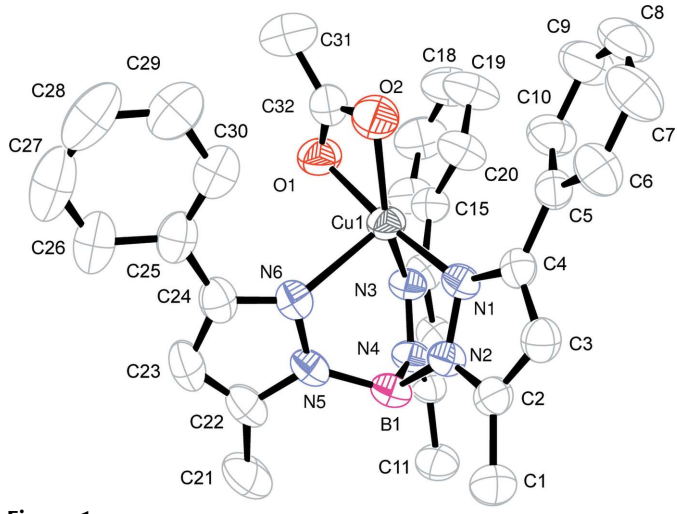


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level. For clarity, all H atoms and the atom labels for C16 and C17 have been omitted.

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References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, P., Fujisawa, K. & Solomon, E. I. (2000). *J. Am. Chem. Soc.* **122**, 10177–10193.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fujisawa, K., Kobayashi, T., Fujita, K., Kitajima, N., Moro-oka, Y., Miyashita, Y., Yamada, Y. & Okamoto, K. I. (2000). *Bull. Chem. Soc. Jpn*, **73**, 1797–1804.
Fujisawa, K., Miyashita, Y., Yamada, Y. & Okamoto, K. I. (2001). *Bull. Chem. Soc. Jpn*, **74**, 1065–1066.
Fujisawa, K., Tada, N., Ishikawa, Y., Higashimura, H., Miyashita, Y. & Okamoto, K. I. (2004). *Inorg. Chem. Commun.* **7**, 209–212.
Keij, F. S., Haasnoot, J. G., Oosterling, A. J., Reedijk, J., O'Connor, C. J. & Zhang, J. H. (1991). *Inorg. Chim. Acta*, **181**, 185–93.
Kitajima, N., Fujisawa, K., Fujimoto, C., Moro-oka, Y., Hashimoto, S., Kitagawa, T., Toriumi, K., Tatsumi, K. & Nakamura, A. (1992). *J. Am. Chem. Soc.* **114**, 1277–1291.
Kitajima, N., Kiyoshi, F. & Moro-oka, Y. (1990). *J. Am. Chem. Soc.* **112**, 3210–3212.
Komiyama, K. F., Furutachi, H., Nagatomo, S., Hashimoto, A., Hayashi, H., Fujinami, S., Suzuki, S. & Kitagawa, T. (2004). *Bull. Chem. Soc. Jpn*, **77**, 59.
Parkin, G. (2004). *Chem. Rev.* **104**, 699–767.
Puert, D. T. & Cohen, S. M. (2002). *Inorg. Chem.* **41**, 5075–5082.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sun, Y.-J., Zhang, L. Z., Cheng, P., Lin, H.-K., Yan, S.-P., Sun, W., Liao, D.-Z., Jiang, Z.-H. & Shen, P.-W. (2003). *Inorg. Chem.* **42**, 508–515.
Wada, A., Honda, Y., Yamaguchi, S., Nagatomo, S., Kitagawa, T., Jitsukawa, K. & Masuda, H. (2004). *Inorg. Chem.* **43**, 5725–5735.