

## Carbonyl[hydrotris(3,5-dimethylpyrazol-1-yl)-borato]copper(I) acetonitrile solvate

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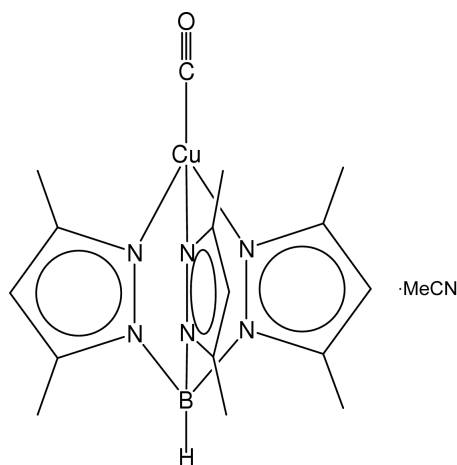
## Key indicators

Single-crystal X-ray study  
T = 150 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
R factor = 0.042  
wR factor = 0.125  
Data-to-parameter ratio = 19.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $[\text{Cu}(\text{C}_{15}\text{H}_{22}\text{BN}_6)(\text{CO})] \cdot \text{C}_2\text{H}_3\text{N}$ , crystallizes as neutral  $[\text{Tp}^*\text{Cu}(\text{CO})]$   $\{[\text{Tp}^*]^- = \text{hydrotris}(3,5\text{-dimethylpyrazol-1-yl})\text{borate}\}$  molecular units and non-coordinated acetonitrile molecules. The distorted tetrahedral coordination geometry of the copper(I) centre comprises the three N atoms of the  $[\text{Tp}^*]^-$  anion [ $\text{Cu}-\text{N}$  2.033 (2)–2.054 (2)  $\text{Å}$ ] and the C atom of the carbon monoxide molecule [ $\text{Cu}-\text{C}$  1.785 (4)  $\text{Å}$ ].

## Comment

The structure of the title compound  $[\text{Tp}^*\text{Cu}(\text{CO})] \cdot \text{MeCN}$   $\{[\text{Tp}^*]^- = \text{hydrotris}(3,5\text{-dimethylpyrazol-1-yl})\text{borate}\}$ , (I), comprises neutral  $[\text{Tp}^*\text{Cu}(\text{CO})]$  molecular units and non-coordinated acetonitrile molecules. The  $[\text{Tp}^*\text{Cu}(\text{CO})]$  molecular unit is similar to those of previously structurally characterized analogues, which differ solely in the identities of the 3,5-substituents on the pyrazole rings (Churchill *et al.*, 1975; Conry *et al.*, 1999; Dias & Kim, 1996; Dias *et al.*, 1996; Imai *et al.*, 1998; Kitajima *et al.*, 1992).



(I)

The copper(I) centre has a distorted tetrahedral geometry comprising the three N atoms of the  $[\text{Tp}^*]^-$  anion and the C atom of the carbon monoxide molecule. The Cu–N and Cu–C interatomic distances [ $\text{Cu}-\text{N}$  2.033 (2)–2.054 (2) and  $\text{Cu}-\text{C}$  1.785 (4)  $\text{Å}$ ] and N–Cu–C and Cu–C–O interatomic angles [ $\text{N}-\text{Cu}-\text{C}$  124.27 (14)–124.52 (14) and  $\text{Cu}-\text{C}-\text{O}$  179.3 (4) $^\circ$ ] fall within the range of values reported previously [ $\text{Cu}-\text{N}$  2.014–2.086,  $\text{Cu}-\text{C}$  1.752–1.808  $\text{Å}$ ,  $\text{N}-\text{Cu}-\text{C}$  119.4–128.5 and  $\text{Cu}-\text{C}-\text{O}$  176.6–180.0 $^\circ$  (Churchill *et al.*, 1975; Conry *et al.*, 1999; Dias & Kim, 1996; Dias *et al.*, 1996; Imai *et al.*, 1998; Kitajima *et al.*, 1992)].

## Experimental

The title compound was prepared following an adaptation of a literature method (Abu Salah *et al.*, 1982).  $\text{Cu}(\text{MeCN})_4\text{BF}_4$  (1.10 g, 3.50 mmol) and  $\text{KTP}^*$  (1.18 g, 3.51 mmol) were dissolved in acetonitrile (200 ml), previously saturated with CO gas. The white solid, formed after stirring for 2 h under a stream of CO gas, was isolated by filtration (1.16 g, 2.69 mmol, 77% yield). A small crop of crystals was obtained from the mother liquor after a further 24 h under CO gas.

### Crystal data

$[\text{Cu}(\text{C}_{15}\text{H}_{22}\text{BN}_6)(\text{CO})]\cdot\text{C}_2\text{H}_3\text{N}$	$D_x = 1.344 \text{ Mg m}^{-3}$
$M_r = 429.80$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2631 reflections
$a = 14.915(2) \text{ \AA}$	$\theta = 2.5\text{--}25.4^\circ$
$b = 7.6811(10) \text{ \AA}$	$\mu = 1.05 \text{ mm}^{-1}$
$c = 18.688(2) \text{ \AA}$	$T = 150(2) \text{ K}$
$\beta = 97.360(2)^\circ$	Plate, colourless
$V = 2123.3(5) \text{ \AA}^3$	$0.30 \times 0.14 \times 0.03 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART1000 CCD area-detector diffractometer	4937 independent reflections
$\omega$ scans	3300 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$R_{\text{int}} = 0.050$
$T_{\text{min}} = 0.854$ , $T_{\text{max}} = 1.000$	$\theta_{\text{max}} = 28.7^\circ$
14745 measured reflections	$h = -19 \rightarrow 19$
	$k = -10 \rightarrow 10$
	$l = -24 \rightarrow 24$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.255P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.125$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.50 \text{ e \AA}^{-3}$
4937 reflections	$\Delta\rho_{\text{min}} = -0.49 \text{ e \AA}^{-3}$
260 parameters	
H-atom parameters constrained	

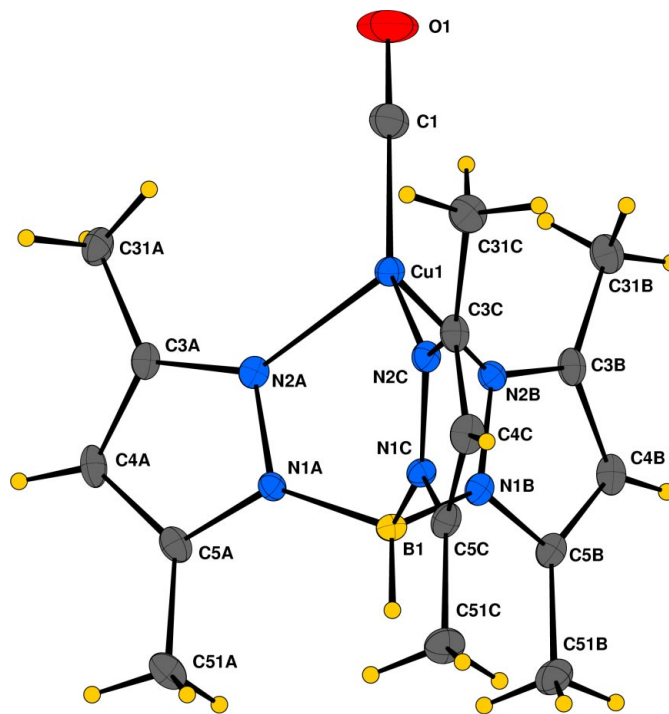
**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cu1—C1	1.785 (4)	Cu1—N2B	2.033 (2)
Cu1—N2A	2.033 (3)	Cu1—N2C	2.054 (2)
		C1—O1	1.125 (4)
C1—Cu1—N2A	124.52 (14)	N2A—Cu1—N2C	91.46 (10)
C1—Cu1—N2B	124.27 (14)	N2B—Cu1—N2C	91.05 (10)
N2A—Cu1—N2B	91.18 (10)	O1—C1—Cu1	179.3 (4)
C1—Cu1—N2C	124.38 (14)		

Methyl H atoms were located from  $\Delta F$  syntheses and refined as part of a rigid rotating group with  $\text{C—H} = 0.96 \text{ \AA}$  and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . After location from  $\Delta F$  syntheses, other H atoms were placed geometrically and refined using a riding model;  $\text{B—H}$  and  $\text{C—H}$  distances were constrained to 0.98 and 0.93  $\text{\AA}$ , respectively, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{B or C})$ .

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT and SHELXTL (Bruker, 1997); program(s) used to solve structure: SIR92 (Altomare *et al.*, 1994); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL and CAMERON (Watkin *et al.*, 1996); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2001).



**Figure 1**

A view of the title compound showing the atom-numbering scheme, but with the non-coordinated acetonitrile solvent molecule omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level.

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