Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[*N*,*N*′-bis(3,3-diphenylprop-2-enylidene)-ethane-1,2-diamine-κ^2N,N']copper(I) triiodide

Aliakbar Dehno Khalaji,[a] Mehdi Amirnasr[a] and Jean-Claude Daran[b]*

[a]Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran, and [b]Laboratoire de Chimie de Coordination, CNRS UPR8241, 205 Route de Narbonne, 31077 Toulouse Cedex, France

Correspondence e-mail: daran@lcc-toulouse.fr

Received 26 October 2006
Accepted 27 October 2006

The title complex, $[Cu(C_{32}H_{28}N_2)_2]I_3$, contains cations having Cu^I coordinated by four N atoms of two *N*,*N*′-bis(3,3-diphenylprop-2-enylidene)ethane-1,2-diamine ($Phca_2en$) ligands in a distorted tetrahedral fashion and isolated linear I_3^- anions. The $Phca_2en$ ligand adopts a *Z*,*Z* conformation and acts as a bidentate ligand coordinating *via* two N atoms to the Cu atom. The Cu and central I atoms are located on twofold axes.

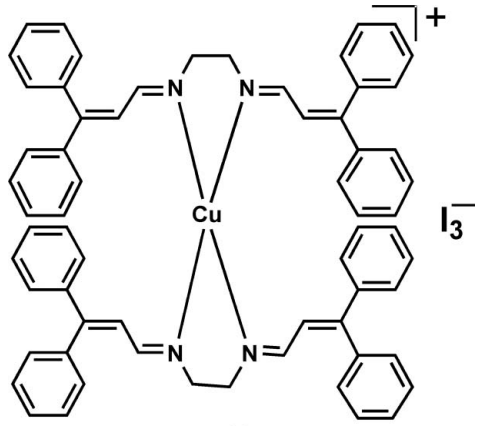
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.069
Data-to-parameter ratio = 28.7

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

Comment

The structural and spectroscopic properties of many Cu^I complexes with bidentate Schiff base ligands have been increasingly studied over recent years (Amirnasr *et al.*, 2006; Khalaji *et al.*, 2006). Depending on the ligands involved, Cu^I complexes can show a wide variety of structures (Kickelbick *et al.*, 2002, 2003; Zhou *et al.*, 2006). In this context, we decided to examine the nature of a Cu^I complex formed with an unconjugated diimine ligand. The title complex, (I), was prepared by reacting the bidentate ligand *N*,*N*′-bis(β-phenylcinnamaldehyde)-1,2-diiminoethane ($Phca_2en$) with CuI.



(I)

The asymmetric unit of (I) contains a $[Cu(Phca_2en)_2]^+$ cation, shown in Fig. 1, and a linear triiodide anion. The Cu and central I atoms are located on twofold axes. Four N atoms of the $Phca_2en$ ligands are coordinated to the Cu^I centre. The $Phca_2en$ ligand chelates the Cu^I atom to form a five-membered ring, with N—Cu—N = 83.67 (11)°, which is in good agreement with the corresponding angles in related complexes (Amirnasr *et al.*, 2006; Khalaji *et al.*, 2006). The Cu—N($Phca_2en$) distance of 2.023 (2) Å is similar to those in the pseudotetrahedral (diimine) Cu^I complexes (Amirnasr *et al.*, 2006; Kickelbick *et al.*, 2002, 2003; Khalaji *et al.*, 2006;

Dehghanpour & Mojahed, 2006). The I—I distance of 2.9182 (3) Å is similar to that observed in the complex $[Mn(phen)_3][I_3]_2$ (2.9255 Å; Horn *et al.*, 2002).

Experimental

The *N*,*N*′-bis(β-phenylcinnamaldehyde)-1,2-diiminoethane ligand, $Phca_2en$, was prepared as reported elsewhere (Amirnasr *et al.*, 2002). Compound (I) was prepared by the reaction of CuI with $Phca_2en$ (molar ratio 1:1) in acetonitrile solution at 298 K. The resulting dark-red precipitate was filtered off and dried under vacuum. Dark-red crystals of (I) were obtained by the slow diffusion of Et_2O vapour into an acetonitrile solution of the complex at 298 K.

Crystal data

$[Cu(C_{32}H_{28}N_2)_2]I_3$
M_r = 1325.38
Tetragonal, $P\bar{4}n2$
a = 17.1304 (7) Å
c = 9.6273 (4) Å
V = 2825.1 (2) Å^3
Z = 2
D_x = 1.558 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.07 mm^{-1}
T = 180 (2) K
Prism, dark red
0.4 × 0.38 × 0.32 mm

Data collection

Oxford Diffraction XCALIBUR diffractometer
φ and ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.678, T_{max} = 0.821 (expected range = 0.426–0.516)
29420 measured reflections
4735 independent reflections
3587 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 32.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.069
S = 1.10
4735 reflections
165 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2 + 1.9967P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}
Absolute structure: Flack (1983) and Bernardinelli & Flack (1985), using 2109 Friedel pairs
Flack parameter: −0.031 (18)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (aromatic H) or 0.99 Å (methylene H) and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

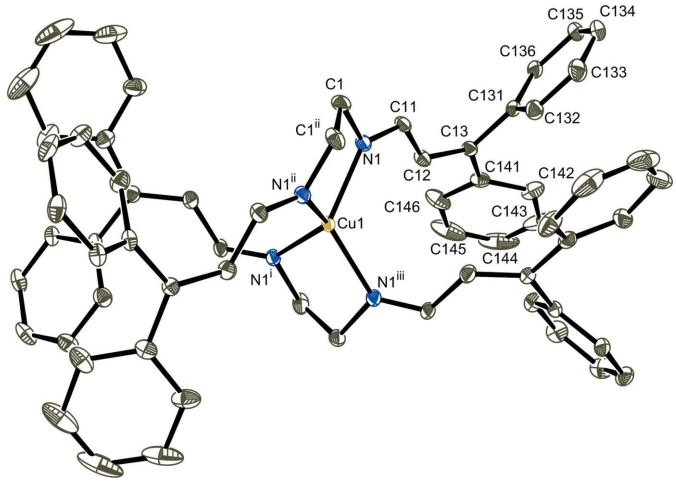


Figure 1
The structure of the $[Cu(Phca_2en)_2]^+$ cation of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms and the I_3^- anion have been omitted for clarity. [Symmetry codes: (i) $-x, -y, z$; (ii) $\frac{1}{2}+y, \frac{1}{2}+x, \frac{1}{2}-z$; (iii) $\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z$].

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Amirnasr, M., Kickelbick, G. & Dehghanpour, S. (2006). *Helv. Chim. Acta*, **89**, 274–732.
Amirnasr, M., Mahmoudkhani, A. H., Gorji, A., Dehghanpour, S. & Bijanzadeh, H. R. (2002). *Polyhedron*, **21**, 2733–2742.
Bernardinelli, G. & Flack, H. D. (1985). *Acta Cryst.* A**41**, 500–511.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Dehghanpour, S. & Mojahed, F. (2006). *Anal. Sci.* **22**, x81–x82.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Horn, C., Berben, L., Chow, H., Scudder, M. & Dance, I. (2002). *CrystEngComm*, **4**, 7–12.
Khalaji, A. D., Amirnasr, M. & Welter, R. (2006). *Anal. Sci.* **22**, x49–x50.
Kickelbick, G., Amirnasr, M., Khalaji, A. D. & Dehghanpour, S. (2002). *Acta Cryst.* E**58**, m381–m382.
Kickelbick, G., Amirnasr, M., Khalaji, A. D. & Dehghanpour, S. (2003). *Aust. J. Chem.* **56**, 323–328.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED* (Version 1.171.31.5). Oxford Diffraction Ltd., Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Zhou, X.-H., Wu, T. & Li, D. (2006). *Inorg. Chim. Acta*, **359**, 1442–1448.