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5,5′-Dimethyl-2,2′-bipyrazine

Chad Eller, Bradley W. Smucker, Robert Kirgan, David M. Eichhorn and D. Paul Rillema*

Department of Chemistry, Wichita State University, KS 67226, USA

Correspondence e-mail: paul.rillema@wichita.edu

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.136
Data-to-parameter ratio = 12.1

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

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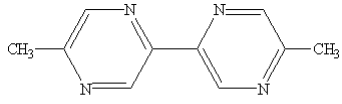
The crystal structure of the title compound, $C_{10}H_{10}N_4$, a molecule synthesized as a dye, was determined by X-ray diffraction at room temperature. The molecule has a center of inversion located midway between the pyrazine units.

Comment

5,5′-Dimethyl-2,2′-bipyrazine, (I), was prepared for attachment to Ru^{II} and Re^{I} atoms, for use as dyes in solid-state regenerative solar-energy cells. The compound acts as a conduit of electrons between the metal centers and the semiconducting dye anchors. The molecule is centrosymmetric, and thus essentially planar.



(I)

Experimental

The title compound was prepared according to the procedures described by Lafferty & Case (1967). 5-Methyl-2-pyrazinoic acid was dissolved in concentrated NH_4OH and the solvent was removed by rotary evaporation, resulting in isolation of the ammonium pyrazinate salt. The solid was dried at 313 K in a vacuum oven and then dissolved in water. A saturated solution of copper(II) acetate was added in the ratio of one copper cation to two pyrazinate anions. The resulting blue–green solid was removed by vacuum filtration, washed with ether and dried at 373 K in a vacuum oven. The copper salt was placed in a pyrolysis vessel and heated between 558 and 584 K, displacing a yellow product that precipitated on the walls of the pyrolysis vessel. The product was dissolved in acetone and recrystallized from ether (yield 6%; m.p. 420 K). ^{1}H NMR ($CDCl_3$): δ 2.595 (*s*, 6H), 8.688 (*s*, 2H), 9.062 (*d*, 2H). Crystals of (I) suitable for X-ray diffraction were grown from an ether solution. The crystal of the compound does not contain any solvent molecules.

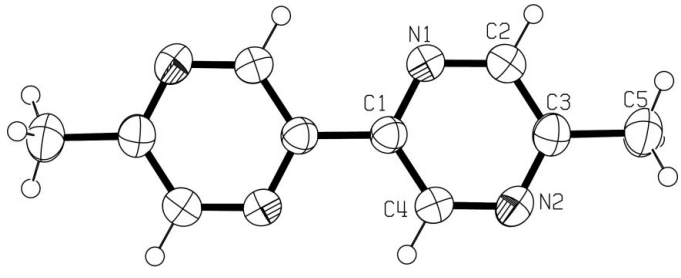


Figure 1
ORTEP-3 (Farrugia, 1997) representation of (I), with displacement ellipsoids at the 50% probability level.

Crystal data

$C_{10}H_{10}N_4$
$M_r = 186.14$
Triclinic, $P\overline{1}$
$a = 3.9580\ (7)$ Å
$b = 5.9476\ (16)$ Å
$c = 10.107\ (2)$ Å
$\alpha = 102.828\ (19)^\circ$
$\beta = 92.100\ (17)^\circ$
$\gamma = 91.27\ (2)^\circ$
$V = 231.72\ (9)$ Å^3
$Z = 1$
$D_x = 1.334$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
$\theta = 10$–12°
$\mu = 0.09$ mm^{-1}
$T = 298\ (2)$ K
Needle, white
0.4 × 0.1 × 0.1 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: ψ-scan (North *et al.*, 1968)
$T_{min} = 0.802$, $T_{max} = 0.989$
1613 measured reflections
811 independent reflections
425 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 25.0^\circ$
$h = -4 \rightarrow 4$
$k = -7 \rightarrow 7$
$l = -11 \rightarrow 11$
3 standard reflections
frequency: 60 min
intensity decay: 10%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.136$
$S = 0.96$
811 reflections
67 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.103P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.036$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

H atoms were placed at calculated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å. The U_{iso}(H) values of the methyl H atoms were taken as $1.5U_{eq}$(C); the U_{iso}(H) values of the other H atoms were refined. The torsion angle of the methyl H atoms was estimated from the electron density, and was allowed to refine.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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