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[2-(3,5-Dimethyl-1*H*-pyrazol-1-yl-κN^2)-1,10-phenanthroline-$\kappa^2 N,N'$]bis(nitrito-$\kappa^2 O,O'$)cadmium(II)

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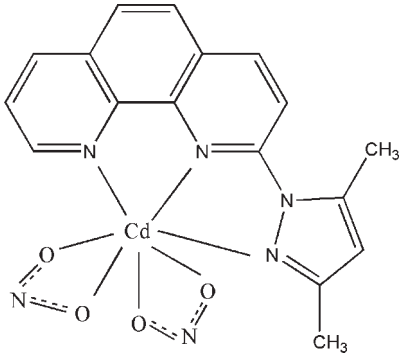
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.032; wR factor = 0.087; data-to-parameter ratio = 13.0.

In the title complex, $[Cd(NO_2)_2(C_{17}H_{14}N_4)]$, the Cd^{II} ion assumes a distorted monocapped octahedral coordination geometry defined by an N_3O_4 donor set. The crystal structure is stabilized by π–π stacking interactions [shortest centroid–centroid distance = 3.5537 (18) Å].

Related literature

For related structures, see: Wang *et al.* (2009); Sun *et al.* (2010).



Experimental

Crystal data

$[Cd(NO_2)_2(C_{17}H_{14}N_4)]$
M_r = 478.74
Triclinic, $P\overline{1}$
a = 10.0306 (15) Å
b = 10.4694 (15) Å
c = 10.5702 (15) Å
α = 67.697 (2)°
β = 83.508 (2)°
γ = 62.326 (2)°
V = 906.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 298 K
0.51 × 0.46 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.570, T_{max} = 0.865
4759 measured reflections
3305 independent reflections
3098 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.087
S = 1.03
3305 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2681).

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