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9,10-Dihydro-7*H*-benzo[*de*]imidazo-[2,1-*a*]isoquinolin-7-one

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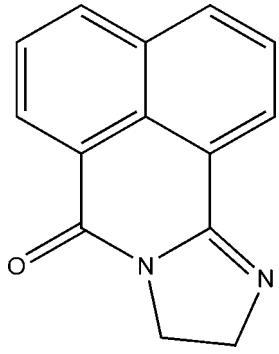
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.008 Å; R factor = 0.075; wR factor = 0.202; data-to-parameter ratio = 11.9.

In the title compound, $C_{14}H_{10}N_2O$, all non-H atoms are essentially coplanar (r.m.s. deviation = 0.013 Å). The crystal structure is stabilized by π–π stacking interactions [centroid–centroid distance = 3.506 (3) Å].

Related literature

For the use of rigid ligands in the formation of metal-organic coordination polymers, see: Chen *et al.* (2006); Yang *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{10}N_2O$
M_r = 222.24
Orthorhombic, $P2_12_12_1$
a = 4.4949 (2) Å
b = 14.9891 (9) Å
c = 15.1357 (8) Å
V = 1019.76 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.20 × 0.05 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.995
8736 measured reflections
1837 independent reflections
1207 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.202
S = 1.01
1837 reflections
154 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2409).

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supplementary materials

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9,10-Dihydro-7*H*-benzo[*de*]imidazo[2,1-*a*]isoquinolin-7-one

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Comment

The title compound, $C_{14}H_{10}N_2O$, (I) can be used as a rigid ligand to form metal-organic coordination polymers, such as $[Ag(C_{14}H_{10}N_2O)(NO_3)]_n$, $[Ag(C_{14}H_{10}N_2O)_2(NO_3)]_n$, $[Ag(C_{14}H_{10}N_2O)_2(BF_4)]_n$ (Yang *et al.*, 2009) and $[Cu_2(CH_3COO)_4(C_{14}H_{10}N_2O)_2]_n$ (Chen *et al.*, 2006). However, the crystal structure of 9,10-dihydro-7*H*-benzo[de]imidazo[2,1-*a*]-isoquinolin-7-one have not been reported so far. We report herein the synthesize and the crystal structure of (I). In the title molecule , $C_{14}H_{10}N_2O$, all non-H atoms are essentially coplanar (r.m.s. 0.013 Å). The crystal structure is stabilized by π–π stacking interactions (centroid -centroid distance 3.506 (3)Å, Cg =C4/C5/C6/C7/C8/C9 ; Cg^i =C4/C5/C6/C7/C8/C9 ; symmetry code (i) x-1, y, z)

Experimental

White prism-shaped single crystals of 9,10-dihydro-7*H*-benzo[de]imidazo[2,1-*a*]-isoquinolin-7-one were initially obtained from the hydrothermal reaction of Naphthalene-1,8-dicarboxylic anhydride (0.3 g), ethylenediamine (5 ml) and H_2O (10 ml) using Teflon lined bomb at 160°C for 5 days and then cooled to room temperature. A few single crystals suitable for X-ray diffraction analysis were obtained.

Refinement

Constraint instruction ′DELU 0.01 C14 N2′ was used in the refinement. The final difference map shows that the highest peak is 0.27 e/Å^3 at 1.55 Å from O(1), while the deepest hole is -0.33 e/Å^3 at 0.16 Å from H(13B). H atoms were placed in geometrically calculated positions with C—H distances in the range 0.93-0.97Å and were refined using a riding model, with $U_{iso}(H)=1.2U_{eq}(C)$. Friedel pairs (715) were merged.

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

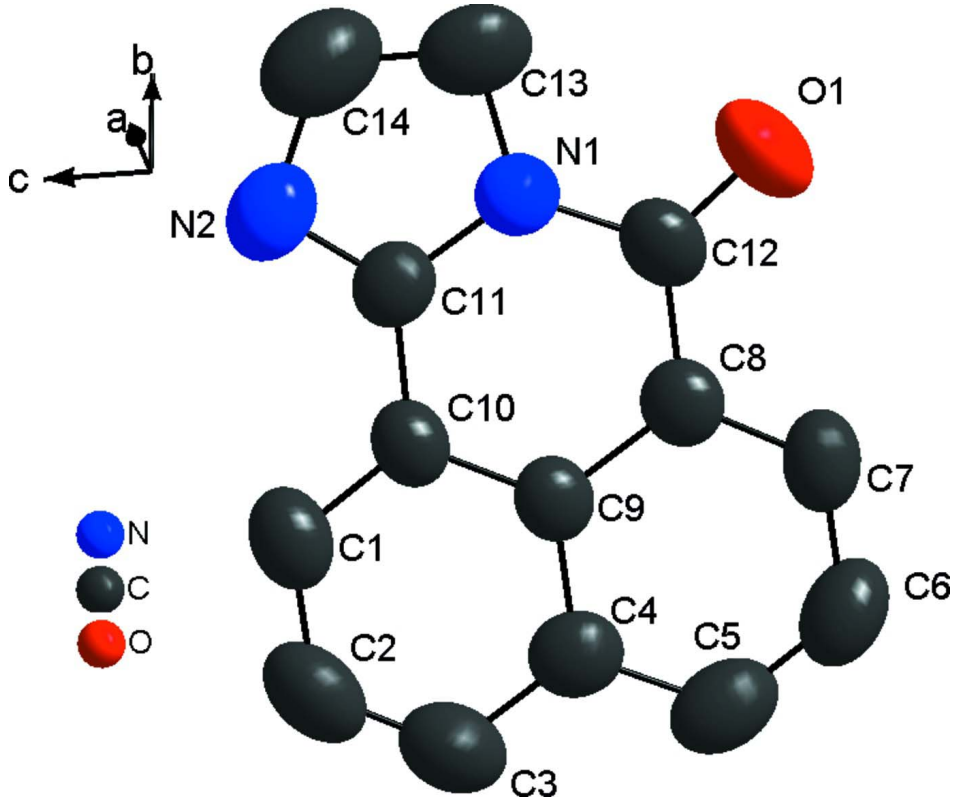

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

9,10-Dihydro-7*H*-benzo[*de*]imidazo[2,1-*a*]isoquinolin-7-one

Crystal data

$C_{14}H_{10}N_2O$
$M_r = 222.24$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.4949$ (2) Å
$b = 14.9891$ (9) Å
$c = 15.1357$ (8) Å
$V = 1019.76$ (9) Å^3
$Z = 4$
$F(000) = 464$
$D_x = 1.448$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 946 reflections
$\theta = 2.7$–$19.8°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Prism, colourless
0.20 × 0.05 × 0.05 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 83.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.982$, $T_{max} = 0.995$
8736 measured reflections
1837 independent reflections
1207 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.9°$
$h = -5 \rightarrow 5$
$k = -18 \rightarrow 16$
$l = -18 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.075$
$wR(F^2) = 0.202$
$S = 1.01$
1837 reflections
154 parameters
1 restraint
1 constraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.9931P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.8099 (9)	0.5958 (3)	0.5858 (3)	0.0586 (11)
C9	0.4344 (11)	0.4484 (3)	0.5830 (3)	0.0526 (11)
C10	0.5848 (10)	0.4693 (3)	0.6615 (3)	0.0537 (11)
C12	0.6647 (12)	0.5790 (3)	0.5059 (3)	0.0614 (14)
C11	0.7765 (11)	0.5470 (3)	0.6614 (3)	0.0556 (11)
C5	0.0907 (13)	0.3543 (4)	0.4989 (4)	0.0772 (17)
H5	−0.0366	0.3055	0.4963	0.093*
C1	0.5498 (12)	0.4169 (4)	0.7347 (3)	0.0692 (14)
H1	0.6487	0.4308	0.7868	0.083*
O1	0.7130 (11)	0.6295 (2)	0.4429 (2)	0.0886 (14)
C8	0.4680 (11)	0.5014 (3)	0.5046 (3)	0.0557 (12)
C4	0.2423 (12)	0.3730 (3)	0.5796 (3)	0.0620 (13)
C7	0.3183 (12)	0.4788 (4)	0.4287 (3)	0.0673 (14)
H7	0.3457	0.5130	0.3781	0.081*
N2	0.9310 (11)	0.5775 (3)	0.7269 (3)	0.0773 (13)
C3	0.2118 (14)	0.3213 (4)	0.6554 (4)	0.0774 (16)
H3	0.0863	0.2720	0.6547	0.093*
C13	1.0057 (13)	0.6648 (3)	0.6011 (4)	0.0778 (17)
H13A	0.9115	0.7223	0.5921	0.093*
H13B	1.1794	0.6604	0.5633	0.093*
C6	0.1267 (13)	0.4058 (4)	0.4255 (4)	0.0805 (17)
H6	0.0242	0.3924	0.3738	0.097*
C2	0.3623 (14)	0.3418 (4)	0.7303 (4)	0.0825 (18)
H2	0.3413	0.3055	0.7797	0.099*
C14	1.0800 (16)	0.6516 (4)	0.6897 (5)	0.100 (2)

H14A	1.0297	0.7048	0.7230	0.120*
H14B	1.2931	0.6425	0.6945	0.120*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.061 (3)	0.056 (2)	0.060 (3)	0.003 (2)	0.006 (2)	−0.006 (2)
C9	0.052 (3)	0.054 (3)	0.051 (3)	0.013 (2)	0.011 (2)	−0.003 (2)
C10	0.050 (2)	0.061 (3)	0.051 (3)	0.012 (2)	0.006 (2)	0.002 (2)
C12	0.068 (3)	0.054 (3)	0.062 (3)	0.016 (3)	0.011 (3)	0.002 (2)
C11	0.047 (3)	0.061 (3)	0.059 (3)	0.010 (3)	0.005 (2)	−0.008 (2)
C5	0.057 (3)	0.079 (4)	0.095 (5)	−0.001 (3)	0.011 (3)	−0.028 (3)
C1	0.066 (3)	0.083 (4)	0.059 (3)	0.018 (3)	0.007 (3)	0.005 (3)
O1	0.118 (3)	0.074 (2)	0.074 (2)	0.006 (3)	0.021 (3)	0.021 (2)
C8	0.050 (3)	0.058 (2)	0.060 (3)	0.014 (2)	0.003 (2)	0.001 (2)
C4	0.051 (3)	0.060 (3)	0.075 (3)	0.009 (3)	0.011 (3)	−0.008 (3)
C7	0.067 (3)	0.081 (4)	0.054 (3)	0.015 (3)	0.000 (3)	−0.004 (3)
N2	0.077 (3)	0.081 (3)	0.074 (3)	0.003 (3)	−0.007 (3)	−0.014 (2)
C3	0.070 (4)	0.067 (3)	0.095 (4)	0.006 (3)	0.023 (3)	0.007 (3)
C13	0.068 (4)	0.059 (3)	0.106 (5)	0.011 (3)	0.019 (3)	−0.020 (3)
C6	0.072 (4)	0.098 (4)	0.072 (4)	0.005 (4)	−0.008 (3)	−0.023 (4)
C2	0.081 (4)	0.084 (4)	0.083 (4)	0.014 (3)	0.019 (3)	0.024 (3)
C14	0.083 (4)	0.097 (5)	0.120 (6)	0.010 (4)	0.015 (4)	−0.041 (4)

Geometric parameters (Å, º)

N1—C11	1.367 (5)	C1—H1	0.9300
N1—C13	1.377 (6)	C8—C7	1.375 (7)
N1—C12	1.397 (6)	C4—C3	1.391 (7)
C9—C10	1.402 (6)	C7—C6	1.392 (7)
C9—C4	1.423 (6)	C7—H7	0.9300
C9—C8	1.436 (6)	N2—C14	1.414 (8)
C10—C1	1.367 (7)	C3—C2	1.355 (8)
C10—C11	1.448 (6)	C3—H3	0.9300
C12—O1	1.236 (5)	C13—C14	1.396 (8)
C12—C8	1.462 (7)	C13—H13A	0.9700
C11—N2	1.295 (6)	C13—H13B	0.9700
C5—C6	1.363 (8)	C6—H6	0.9300
C5—C4	1.426 (7)	C2—H2	0.9300
C5—H5	0.9300	C14—H14A	0.9700
C1—C2	1.408 (8)	C14—H14B	0.9700
C11—N1—C13	109.4 (4)	C9—C4—C5	118.5 (5)
C11—N1—C12	125.2 (4)	C8—C7—C6	121.7 (5)
C13—N1—C12	125.4 (5)	C8—C7—H7	119.2
C10—C9—C4	120.1 (4)	C6—C7—H7	119.2
C10—C9—C8	121.7 (4)	C11—N2—C14	103.1 (5)
C4—C9—C8	118.2 (4)	C2—C3—C4	121.0 (6)
C1—C10—C9	120.2 (5)	C2—C3—H3	119.5
C1—C10—C11	122.1 (5)	C4—C3—H3	119.5

C9—C10—C11	117.8 (4)	N1—C13—C14	102.0 (5)
O1—C12—N1	118.4 (5)	N1—C13—H13A	111.4
O1—C12—C8	125.7 (5)	C14—C13—H13A	111.4
N1—C12—C8	116.0 (4)	N1—C13—H13B	111.4
N2—C11—N1	113.1 (4)	C14—C13—H13B	111.4
N2—C11—C10	127.0 (5)	H13A—C13—H13B	109.2
N1—C11—C10	119.8 (4)	C5—C6—C7	119.3 (5)
C6—C5—C4	122.0 (6)	C5—C6—H6	120.3
C6—C5—H5	119.0	C7—C6—H6	120.3
C4—C5—H5	119.0	C3—C2—C1	121.3 (5)
C10—C1—C2	119.3 (5)	C3—C2—H2	119.3
C10—C1—H1	120.3	C1—C2—H2	119.3
C2—C1—H1	120.3	C13—C14—N2	112.4 (6)
C7—C8—C9	120.2 (5)	C13—C14—H14A	109.1
C7—C8—C12	120.3 (5)	N2—C14—H14A	109.1
C9—C8—C12	119.6 (4)	C13—C14—H14B	109.1
C3—C4—C9	118.1 (5)	N2—C14—H14B	109.1
C3—C4—C5	123.4 (6)	H14A—C14—H14B	107.9