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## Pyridine-4-carbaldehyde azine

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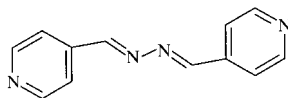
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In the crystal structure of the title compound, C<sub>12</sub>H<sub>10</sub>N<sub>4</sub>, the pyridine ring makes a dihedral angle of 1.12 (9)° with the mean plane of the complete almost planar and crystallographically centrosymmetric molecule. There are stacks of parallel molecules along the *a*-axis direction, with alternate stacks having a herring-bone arrangement relative to each other and an interplanar spacing of 3.551 Å.

### Comment

The title compound, (I), is known not only as a coordinating reagent to determine the concentration of the Fe<sup>II</sup> ion in solution (Luque de Castro & Valcarcel, 1978), but also as a precursor in the atactic polymerization of 4-vinylpyridine (Biedermann *et al.*, 1972). In addition, this Schiff base ligand derived from hydrazine finds a wide range of applications in coordination chemistry owing to its polydentate chelating ability (Tarafder & Khan, 1991). Although the synthesis and characterization of 4,4'-azinodimethyldipyridine and the crystal structure of its diperchlorate salt, C<sub>12</sub>H<sub>10</sub>N<sub>4</sub><sup>2+</sup>·2ClO<sub>4</sub><sup>-</sup>, have been reported (Chen *et al.*, 1997), the crystal structure of 4,4'-azinodimethyldipyridine or pyridine-4-carbaldehyde azine, (I), has not been reported. The title compound acts as a potential bridging ligand in the study of supramolecular chemistry and can coordinate to metal ions to form multi-dimensional structures.



(I)

There is half a molecule in the asymmetric unit and the other half is inversion related. The bond distances and angles agree with those of the perchlorate salt (Chen *et al.*, 1997). The C6=N2 distance is shorter than 1.285 (7) Å and the bond

angles C6—N2—N2<sup>i</sup> [symmetry code: (i) 1 - *x*, 2 - *y*, 1 - *z*] and C1—C6—N2 are slightly smaller than those of 112.2 (2) and 120.7 (2)°, respectively, reported for 2,2'-azinodimethyldiphenol (Xu *et al.*, 1994). The molecule adopts an antiperiplanar conformation with respect to the N2—N2<sup>i</sup> bond. Atoms C6 and C6<sup>i</sup> are in a *trans* orientation with respect to the N2—N2<sup>i</sup> bond. The pyridine ring makes a dihedral angle of 1.12 (9)° with the mean plane of the complete almost planar molecule. There are stacks of parallel molecules along the *a*-axis direction, with alternate stacks having a herring-bone arrangement relative to each other with an interplanar spacing of 3.551 Å.

### Experimental

The title compound was prepared by stirring hydrazine hydrate (80%) and pyridine-4-carboxaldehyde under flowing N<sub>2</sub> in anhydrous EtOH solution at 353 K for 6 h. The solution was then cooled and filtered. The filtrate was evaporated at room temperature for a few weeks and orange block-shaped crystals were obtained.

#### Crystal data

C <sub>12</sub> H <sub>10</sub> N <sub>4</sub>	<i>D<sub>x</sub></i> = 1.293 Mg m <sup>-3</sup>
<i>M<sub>r</sub></i> = 210.24	Mo <i>K</i> α radiation
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Cell parameters from 2605 reflections
<i>a</i> = 3.8515 (3) Å	<i>θ</i> = 2.45–28.32°
<i>b</i> = 11.0201 (8) Å	<i>μ</i> = 0.083 mm <sup>-1</sup>
<i>c</i> = 12.7303 (9) Å	<i>T</i> = 293 (2) K
<i>β</i> = 92.312 (2)°	Block, orange
<i>V</i> = 539.88 (7) Å <sup>3</sup>	0.38 × 0.36 × 0.32 mm
<i>Z</i> = 2	

#### Data collection

Siemens SMART CCD area-detector diffractometer	<i>R</i> <sub>int</sub> = 0.031
<i>ω</i> scans	<i>θ</i> <sub>max</sub> = 28.42°
3584 measured reflections	<i>h</i> = -5 → 5
1325 independent reflections	<i>k</i> = -14 → 7
1065 reflections with <i>I</i> > 2σ( <i>I</i> )	<i>l</i> = -16 → 16

#### Refinement

Refinement on <i>F</i> <sup>2</sup>	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F<sub>o</sub></i> <sup>2</sup> ) + (0.0958 <i>P</i> ) <sup>2</sup> + 0.1438 <i>P</i> ]
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.067	where <i>P</i> = ( <i>F<sub>o</sub></i> <sup>2</sup> + 2 <i>F<sub>c</sub></i> <sup>2</sup> )/3
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.110	(Δ <i>ρ</i> /σ) <sub>max</sub> < 0.001
<i>S</i> = 1.247	Δ <i>ρ</i> <sub>max</sub> = 0.31 e Å <sup>-3</sup>
1325 reflections	Δ <i>ρ</i> <sub>min</sub> = -0.20 e Å <sup>-3</sup>
93 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (Å, °).

N1—C4	1.332 (3)	N2—C6	1.266 (3)
N1—C3	1.337 (3)	N2—N2 <sup>i</sup>	1.407 (3)
C4—N1—C3	116.7 (2)	C6—N2—N2 <sup>i</sup>	112.2 (2)

Symmetry code: (i) 1 - *x*, 2 - *y*, 1 - *z*.

All the H atoms were located from the difference Fourier map and were refined isotropically.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine

structure: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

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