Data Article

2-(1,3-Oxazolin-2-yl)pyridine and 2,6-bis (1,3-oxazolin-2-yl) pyridine

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ABSTRACT

The data presented in this article are related to research articles “Titanium and vanadium catalysts with oxazoline ligands for ethylene-norbornene (co)polymerization (Ochędzam-Siodłak et al., 2018). For the title compounds, 2-(1,3-oxazolin-2-yl)pyridine (Py-ox) and 2,6-bis(1,3-oxazolin-2-yl)pyridine (Py-box), the single-crystal X-ray diffraction measurement together with NMR, GC, MS, DSC analysis, like also the method of crystallization are presented.

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Specifications table

| Subject area               | Chemistry                          |
|----------------------------|------------------------------------|
| More specific subject area | Organic Chemistry, Ligands for Catalysts |
| Type of data               | Figures, tables, text file.         |
|                           | X-ray (table, figures), GC–MS (Figures), 13C NMR (figures), DSC (figures), synthesis (text) |

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How data was acquired
X-ray (Xcalibur diffractometer), NMR (Bruker Ultrashield spectrometer 400 MHz, solvent DMSO-d6), GC–MS (Hewlett Packard HP7890 A GC system), DSC (2010 TA calorimeter)

Data format
X-ray (analyzed), GC–MS (raw), NMR (raw), DSC (raw)

Experimental factors
Crystallization at room temperature. Py-ox - highly anhydrous toluene/hexane mixture, Py-box - DMSO-d6 in NMR tube.

Experimental features
Highly anhydrous condition for crystals are required.

Data source location
City: Opole, Country: Poland, Latitude: N 50°40'23.981", Longitude: E 17°55'53.173', (Lat,Long: 50.673328, 17.93143699999996),

Data accessibility
The Cambridge Crystallographic Data Centre no. CCDC 1815355 and CCDC 1580983 (http://www.ccdc.cam.ac.uk/conts/retrieving.html, email: deposit@ccdc.cam.ac.uk.).

Value of the data
- X-Ray structural information for Py-ox and Py-box compounds not coordinated by metal atom is presented.
- Conformation and association pattern in the crystal state is shown.
- Crystallization methods are shown.
- Purification for Py-ox is improved.

1. Data

The presented compounds, 2-(1,3-oxazolin-2-yl)pyridine (Py-ox) and 2,6-bis(1,3-oxazolin-2-yl)pyridine (Py-box), are commonly applied as ligands for complexes with transition metals: cobalt [2], rhenium [3], platinum and palladium [4,5] for Py-ox, as well as copper [6,7], ruthenium [8–11], rhodium [12], manganese [13], silver [14], nickel [15], cobalt [16], terbium [17], and iron [18], in the case of Py-box. Some of them reveal catalytic properties. In our work, the Py-ox and Py-box compounds were applied as ligands for titanium and vanadium complexes, which turned out to be active in polymerization of ethylene and copolymerization of ethylene with norbornene [1]. The X-Ray information for Py-ox and Py-box compounds can be important for comparative studies, to show differences between these compounds not coordinated by metal atom and applied as ligands. It can help to understand dependence between the structure and activity of the designed complexes. The presented crystallization methods are worth to notice. The improved method of purification enable to obtain the studied compound of high quality.

2. Experimental design, materials and methods

2.1. Synthesis

2.1.1. 2-(1,3-oxazolin-2-yl)pyridine (Py-ox)

The synthesis was performed mainly according to Stokes et al. [19]. The crude product was subjected to flash chromatography using the MeOH: AcOEt (1:4) mixture as eluent. Yield 60%. Elemental analysis C_{8}H_{8}N_{2}O results: calculated C 64.85%, H 5.44%, N 18.91%, experimental C 64.92%, H 5.45%, N 19.09%. $^{1}$H NMR (400 MHz, DMSO-d6) δ 8.65 (1H, J = 4.5 Hz, d), 7.99 (1H, J = 8.0 Hz, d), 7.93 (1H, J = 7.8 Hz, td), 7.54 (1H, m), 4.45 (2H, J = 9.6 Hz, t), 4.00 (2H, J = 9.6 Hz, t). $^{13}$C NMR (400 MHz, DMSO-d6) δ 162.98, 149.53, 146.52, 137.09, 125.90, 123.80, 67.66, 54.61. GC–MS M $^{+}$ 148 m/e. Melting temperature 57.0 (54.6–60.0) °C.
2.1.2. 2,6-bis(1,3-oxazolin-2-yl)pyridine (Py-box)

The synthesis was performed mainly according to Zhu et al. [20]. Yield 76%. Elemental analysis C_{11}H_{11}N_{3}O_{2} results: calculated C 64.82%, H 5.10%, N 19.34%, experimental: C 64.88%, H 5.12%, N 19.39%. 

^{1}H NMR (400 MHz, DMSO-d6) \( \delta \) 8.11 (2H, \( J_{1} \) = 1.2 Hz, \( J_{2} \) = 7.2 Hz, t), 8.02 (1H, \( J_{1} \) = 6.4 Hz, \( J_{2} \) = 2.4 Hz, q), 4.45 (4H, \( J \) = 9.6 Hz, t), 4.01 (4H, \( J \) = 9.6 Hz, t). 

^{13}C NMR (400 MHz, DMSO-d6) \( \delta \) 163.10, 147.01, 138.46, 126.00, 68.28, 55.13. GC–MS M^{+} 217 m/e. Melting temperature 160.6 (159.4–163.0) °C.

2.2. Crystallization

2.2.1. 2-(1,3-oxazolin-2-yl)pyridine (Py-ox)

The crystals were obtained at room temperature from highly anhydrous toluene/hexane mixture. The solvents were freshly distilled over sodium. The highly anhydrous conditions are crucial. All operations were performed in a glove-box filled with argon. Py-ox (20 mg) was placed in a 5 ml snap cap vial with plastic cap and dissolved in toluene (1 ml). Then, hexane (1 ml) was added and the solution was left to stand at room temperature for a week.

2.2.2. 2,6-bis(1,3-oxazolin-2-yl)pyridine (Py-box)

The crystals of appropriate quality were obtained at room temperature from DMSO-d6 solution by long standing time in NMR tube. All operations were performed in a glove-box filled with argon. DMSO-d6 solvent from sealed glass ampoules was applied. Py-box (15 mg) and DMSO-d6 (0.6 ml) was placed in NMR tube and the cap was sealed by a parafilm. The solution was left to stand at room temperature for a month.

2.3. X-ray

The single-crystal X-ray diffraction experiments were performed at 293.0(1)K on the Xcalibur diffractometer, equipped with a CCD area detector and a graphite monochromator for the MoK\( \alpha \)
radiation. The reciprocal space was explored by \( \omega \) scans with detector positions at 60 mm distance from the crystal. The diffraction data processing of studied compounds (Lorentz and polarization corrections were applied) were performed using the CrysAlis CCD [21,22]. Both structures Py-ox and Py-box were solved in the C2 and P2/n space group respectively, by direct methods and refined by a

**Fig. 2.** Association of molecule in the crystal structure. Hydrogen contacts are marked by dashed lines. The numbers of atoms and distances are omitted for clarity. All geometric parameters are in Table 2.

**Fig. 3.** The crystal packing scheme of the title compounds. A view along the c axis of the crystals packing.
### Table 1
X-ray experimental details for 2-(1,3-oxazolin-2-yl)pyridine (Py-ox) and 2,6-bis(1,3-oxazolin-2-yl) pyridine (Py-box).

|                      | Py-ox                          | Py-box                          |
|----------------------|--------------------------------|---------------------------------|
| Chemical formula     | C_8H_8N_2O                     | C_{11}H_{12}N_3O_2              |
| M_r                 | 148.16                         | 217.23                          |
| Crystal system, space group | Monoclinic, C2 | Monoclinic, P2/n |
| a, b, c (Å)        | 10.2571 (7), 10.0159 (6), 14.4647 (9) | 6.4904 (8), 6.5835 (11), 11.9080 (19) |
| β (°)              | 97.497 (6)                     | 94.215 (13)                     |
| V (Å³)             | 1473.31 (16)                   | 507.45 (13)                     |
| Z                  | 8                             | 2                               |
| Measurement temperature | 293.0(1)                      | 293.0(1)                        |
| µ (mm⁻¹)           | 0.09                           | 0.10                            |
| Crystal size (mm)  | 0.4 × 0.3 × 0.2                | 0.5 × 0.4 × 0.3                 |
| Crystal colour     | Colourless                     |                                 |
| Crystal description | Plate                          |                                 |
| Data collection    |                                |                                 |
| Radiation wavelength | 0.71073                        |                                 |
| Radiation type     | MoKα                           |                                 |
| Source             | fine-focus sealed tube         |                                 |
| Measurement device type | Xcalibur                     |                                 |
| Detector area resolution | 1024 × 1024 with blocks 2 × 2 |                                 |
| Absorption correction | –                             |                                 |
| No. of measured, independent and observed | 5,034, 2786, 1587 | 3,172, 993, 459 |
| | reflections |                                |                                 |
| R_{int}            | 0.018                          | 0.048                           |
| (sin θ/λ)_{max} (Å⁻¹) | 0.617                         | 0.616                           |
| Refinement         |                                |                                 |
| R(F^2) > 2σ(F^2), wR(F^2), S | 0.030, 0.077, 0.86 | 0.057, 0.173, 0.87 |
| No. of reflections  | 2786                           | 993                             |
| No. of parameters  | 200                            | 75                              |
| No. of restraints  | 1                              | 0                               |
| Δρ_{max}, Δρ_{min} (e Å⁻³) | 0.11, –0.09 | 0.22, –0.18 |

### Table 2
Selected geometric parameters (Å, °) for Py-ox and Py-box molecules.

#### Structure 2 (Py-ox)

| N1A-C2A | 1.386 (7) | C5B-H5B | 0.9300 |
| N1A-C6A | 1.394 (6) | C7A-N8A | 1.292 (7) |
| C2A-C3A | 1.367 (8) | C7A-O11A | 1.314 (6) |
| C2A-H2A | 0.9300 | C6B-C7B | 1.478 (7) |
| N1B-C6B | 1.360 (6) | N8A-C9A | 1.423 (7) |
| N1B-C2B | 1.393 (7) | C7B-N8B | 1.289 (6) |
| C3A-C4A | 1.400 (8) | C7B-O11B | 1.292 (7) |
| C3A-H3A | 0.9300 | C9A-C10A | 1.518 (8) |
| C2B-C3B | 1.344 (9) | C9A-H9AA | 0.9700 |
| C2B-H2B | 0.9300 | C9A-H9AB | 0.9700 |
| C4A-C5A | 1.307 (8) | N8B-C9B | 1.427 (7) |
| C4A-H4A | 0.9300 | C10A-O11A | 1.470 (7) |
| C3B-C4B | 1.361 (9) | C10A-H10A | 0.9700 |
| C3B-H3B | 0.9300 | C10A-H10B | 0.9700 |
| C5A-C6A | 1.335 (6) | C9B-C10B | 1.513 (8) |
| C5A-H5A | 0.9300 | C9B-H9BA | 0.9700 |
| C4B-C5B | 1.345 (7) | C9B-H9BB | 0.9700 |
| C4B-H4B | 0.9300 | O11B-C10B | 1.488 (6) |
| C6A-C7A | 1.464 (7) | C10B-H10C | 0.9700 |
| C5B-C6B | 1.342 (6) | C10B-H10D | 0.9700 |
| C2A-N1A-C6A | 116.2 (5) | C5B-C6B-C7B | 119.1 (5) |
### Table 2 (continued)

#### Structure 2 (Py-ox)

| Bond/Angle | Structure 2 (Py-ox) | Structure 1 (Py-Box) |
|------------|---------------------|----------------------|
| C3A-C2A-N1A | 122.5 (6)           | N1B-C6B-C7B          |
| C3A-C2A-H2A | 118.8               | C7A-N8A-C9A          |
| N1A-C2A-H2A | 118.8               | N8B-C7B-O11B         |
| C6B-N1B-C2B | 115.8 (5)           | N8B-C7B-C6B          |
| C2A-C3A-C4A | 116.1 (6)           | O11B-C7B-C6B         |
| C2A-C3A-H3A | 122.0               | N8A-C9A-C10A         |
| C4A-C3A-H3A | 122.0               | N8A-C9A-H9AA         |
| C3B-C2B-N1B | 121.2 (6)           | C10A-C9A-H9AA        |
| C3B-C2B-H2B | 119.4               | N8A-C9A-H9AB         |
| N1B-C2B-H2B | 119.4               | C10A-C9A-H9AB        |
| C5A-C4A-C3A | 123.3 (6)           | H9AA-C9A-H9AB        |
| C5A-C4A-H4A | 118.3               | C7B-N88-C9B          |
| C3A-C4A-H4A | 118.3               | O11A-C10A-C9A        |
| C2B-C3B-C4B | 120.0 (6)           | O11A-C10A-H10A       |
| C2B-C3B-H3B | 120.0               | C9A-C10A-H10A        |
| C4B-C3B-H3B | 120.0               | O11A-C10A-H10B       |
| C4A-C5A-C6A | 119.6 (6)           | C9A-C10A-H10B        |
| C4A-C5A-H5A | 120.2               | H10A-C10A-H10B       |
| C6A-C5A-H5A | 120.2               | N88-C9B-C10B         |
| C5B-C4B-C3B | 120.2 (6)           | N88-C9B-H9BA         |
| C5B-C4B-H4B | 119.9               | C10B-C9B-H9BA        |
| C3B-C4B-H4B | 119.9               | N88-C9B-H9BB         |
| C5A-C6A-N1A | 122.4 (5)           | C10B-C9B-H9BB        |
| C5A-C6A-C7A | 118.1 (5)           | H9BA-C9B-H9BB        |
| N1A-C6A-C7A | 119.6 (5)           | C7A-O11A-C10A        |
| C6B-C5B-C4A | 119.1 (5)           | C7B-O11B-C10B        |
| C6B-C5B-H5B | 120.5               | O11B-C10B-C9B        |
| C4B-C5B-H5B | 120.5               | O11B-C10B-H10C       |
| N8A-C7A-O11A | 118.1 (5)         | C9B-C10B-H10C        |
| N8A-C7A-C6A | 122.8 (5)           | O11B-C10B-H10D       |
| O11A-C7A-C6A | 119.1 (6)          | C9B-C10B-H10D        |
| C5B-C6B-N1B | 123.6 (5)           | H10C-C10B-H10D       |

**Symmetry code(s):** (i) \(-x+1/2, y, -z+1/2\).

### Structure 1 (Py-Box)

| Bond/Angle | Structure 2 (Py-ox) | Structure 1 (Py-Box) |
|------------|---------------------|----------------------|
| N1-C2      | 1.355 (3)           | C5-O9                |
| N1-C2      | 1.355 (3)           | N6-C7                |
| C2-C3      | 1.381 (4)           | C7-C8                |
| C2-C5      | 1.468 (4)           | C7-H7A               |
| C3-C4      | 1.380 (4)           | C7-H7B               |
| C3-H3      | 0.9300              | C8-O9                |
| C4-C3\(^i\) | 1.380 (4)          | C8-H8A               |
| C4-H4      | 0.9300              | C8-H8B               |
| C5-N6      | 1.293 (3)           | N6-C7-C8             |
| C2\(^i\)-N1-C2 | 116.0 (4)       | N6-C7-C8             |
| N1-C2-C3   | 123.4 (3)           | N6-C7-H7A            |
| N1-C2-C5   | 116.5 (3)           | C8-C7-H7A            |
| C3-C2-C5   | 120.0 (2)           | N6-C7-H7B            |
| C4-C3-C2   | 119.5 (3)           | C8-C7-H7B            |
| C4-C3-H3   | 120.2               | H7A-C7-H7B           |
| C2-C3-H3   | 120.2               | O9-C8-C7             |
| C3\(^i\)-C4-C3 | 118.1 (4)     | O9-C8-H8A            |
| C3\(^i\)-C4-H4 | 121.0             | C7-C8-H8A            |
| C3-C4-H4   | 121.0               | O9-C8-H8B            |
| N6-C5-O9   | 118.1 (2)           | C7-C8-H8B            |
| N6-C5-C2   | 121.0 (3)           | H8A-C8-H8B           |
| O9-C5-C2   | 120.9 (2)           | C5-O9-C8             |
| C5-N6-C7   | 106.9 (2)           |                      |

\(^i\) Symmetry code(s): (i) \(-x+1/2, y, -z+1/2\).
full-matrix least-squares method using SHELXL14 program [23,24]. The H atoms were found based on geometrical parameters. In both structures H atoms were refined using a riding model. The structure drawings were prepared using SHELXTL and Mercury programs [25] (Figs. 1–3 and Tables 1,2).

### 2.3.1. 2-(1,3-oxazolin-2-yl)pyridine (Py-ox)

#### checkCIF/PLATON report

Structure factors have been supplied for datablock(s) bd203_c

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No syntax errors found. CIF dictionary Interpreting this report

**Datablock: bd203_c**

| Bond precision: C-C = 0.0084 A | Wavelength=0.71073 |
|-------------------------------|---------------------|
| Cell:                         |                     |
| a=10.2571(7)                 | b=10.0159(6)        |
| c=14.4647(9)                 |                     |
| alpha=90                     | beta=97.497(6)      |
| gamma=90                     |                     |
| Temperature: 293 K            |                     |
|                              |                     |
| Calculated Volume 1473.32(16) | Reported Volume 1473.31(16) |
| Space group C 2               | C 2                 |
| Hall group C 2y               | C 2y                |
| Moiety formula C8 H8 N2 O     | C8 H8 N2 O          |
| Sum formula C8 H8 N2 O        | C8 H8 N2 O          |
| Mr 148.16                     | 148.16              |
| Dx,g cm⁻³ 1.336               | 1.336               |
| Z 8                           | 8                   |
| Mu (mm⁻³) 0.092               | 0.092               |
| F000 624.0                    | 624.0               |
| F000’ 624.25                  |                     |
| h,k,l max 12,12,17            | 12,12,17            |
| Nref 2899[1538]               | 2786                |
| Tmin,Tmax 0.997,0.998         |                     |
| Tmin’ 0.996                   |                     |

Correction method= Not given

Data completeness 1.81/0.96 θ(max)= 25.997

R(reflections)= 0.0304(1587) wR2(reflections)= 0.0771(2786)

S = 0.863 Npar= 200

The following ALERTS were generated. Each ALERT has the format test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.
### Alert level B

| Description                                                                 | Value  |
|----------------------------------------------------------------------------|--------|
| PLAT111_ALERT_2_B ADDSYM Detects New (Pseudo) Centre of Symmetry            | 100 %Fit |
| PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem                    | 100 %Fit |
| PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group           | C2/c Check |
| PLAT230_ALERT_2_B Hirshfeld Test Diff for N8B --C7B                          | 8.3 s.u. |
| PLAT230_ALERT_2_B Hirshfeld Test Diff for N8B --C9B                          | 8.2 s.u. |

### Alert level C

| Description                                                                 | Value  |
|----------------------------------------------------------------------------|--------|
| STRVA01_ALERT_4_C Flack parameter is too small                             |        |
| From the CIF: _refine_ls_abs_structure_Flack -1.100                       |        |
| From the CIF: _refine_ls_abs_structure_Flack_su 1.000                     |        |
| PLAT230_ALERT_2_C Hirshfeld Test Diff for O11A --C10A                      | 5.2 s.u. |
| PLAT230_ALERT_2_C Hirshfeld Test Diff for N8A --C7A                        | 5.2 s.u. |
| PLAT230_ALERT_2_C Hirshfeld Test Diff for C3A --C4A                        | 7.0 s.u. |
| PLAT230_ALERT_2_C Hirshfeld Test Diff for O11B --C10B                      | 5.8 s.u. |
| PLAT234_ALERT_4_C Large Hirshfeld Difference N8A --C9A                    | 0.17 Ang. |
| PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of O11A Check |        |
| PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of N1A Check |        |
| PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of C9A Check |        |
| PLAT241_ALERT_2_C High ‘MainMol’ Ueq as Compared to Neighbors of O11B Check|        |
| PLAT242_ALERT_2_C Low ‘MainMol’ Ueq as Compared to Neighbors of C10A Check |        |
| PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds                         | 0.00842 Ang. |
| PLAT411_ALERT_2_C Short Inter H...H Contact H3A ...H3A                    | 2.12 Ang. |
| 1-x,y,1-z = 2_656 Check                                                   |        |
| PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & Stth/L= 0.600           | 2 Report |
| PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.        | 0 Info  |

### Alert level G

| Description                                                                 | Value  |
|----------------------------------------------------------------------------|--------|
| PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High           | 1.000 Report |
| PLAT199_ALERT_3_G Reported _cell_measurement_temperature ...... (K)         | 293 Check |
| PLAT200_ALERT_3_G Reported _diffrn_ambient_temperature ...... (K)           | 293 Check |
| PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O11A                  | 106.8 Degree |
| PLAT399_ALERT_2_G Deviating C-O-C Angle From 120 for O11B                  | 106.0 Degree |
| PLAT720_ALERT_2_G Number of Unusual/Non-Standard Labels                    | 4 Note  |
| PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         | 3 Note  |

**Alert level**

- **A**: Most likely a serious problem - resolve or explain
- **B**: A potentially serious problem, consider carefully
- **C**: Check. Ensure it is not caused by an omission or oversight
- **G**: General information/check it is not something unexpected

**Alert type**

- **1**: CIF construction/syntax error, inconsistent or missing data
- **2**: Indicator that the structure model may be wrong or deficient
- **3**: Indicator that the structure quality may be low
- **4**: Improvement, methodology, query or suggestion
- **5**: Informative message, check
2.3.2. 2,6-bis(1,3-oxazolin-2-yl)pyridine (Py-box)

**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) BD162_a

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No syntax errors found.  CIF dictionary  Interpreting this report

**Datablock: BD162_a**

| Bond precision: C-C | 0.0045 Å | Wavelength | 0.71073 |
|---------------------|----------|------------|---------|
| Cell:               | a=6.4904(8) | b=6.5835(11) | c=11.9080(19) |
| alpha=90            | beta=94.215(13) | gamma=90 |
| Temperature:        | 293 K    |            |         |
|                     |          |            |         |
| Volume              | 507.45(13) | 507.45(13) |         |
| Space group         | P 2/n    | P 2/n      |         |
| Hall group          | -P 2yac  | -P 2yac    |         |
| Moiety formula      | C11 H11 N3 O2 |     | C11 H11 N3 O2 |
| Sum formula         | C11 H11 N3 O2 | C11 H11 N3 O2 | |
| Mr                  | 217.23   | 217.23     |         |
| Dx, g cm⁻³          | 1.422    | 1.422      |         |
| Z                   | 2        | 2          |         |
| Mu (mm⁻¹)           | 0.101    | 0.101      |         |
| F000                | 228.0    | 228.0      |         |
| F000’               | 228.10   |            |         |
| h,k,lmax            | 8,8,14   | 8,8,14     |         |
| Nref                | 992      | 993        |         |
| Tmin, Tmax          | 0.995, 0.997 | 0.995     |
| Tmin’               | 0.995    |            |         |

Correction method= Not given

Data completeness= 1.001  Theta(max)= 25.982

R(reflections)= 0.0572(459)  wR2(reflections)= 0.1732(993)

S = 0.870  Npar= 75

The following ALERTS were generated. Each ALERT has the format  
`test-name_ALERT_alert-type_alert-level`.  
Click on the hyperlinks for more details of the test.
Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 46 %
PLAT241_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of 09 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.7 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ............. 0.0045 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ...... 13.338 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ...... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ...... (K) 293 Check
PLAT398_ALERT_2_G Deviating C-O-C Angle from 120 Deg for O9 105.9 Degree
PLAT953_ALERT_1_G Reported (CIF) and Actual (FCF) Hmax Differ by . 1 Units

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
5 ALERT level G = General information/check it is not something unexpected
3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock BD162_a - ellipsoid plot

Prob = 50
Temp = 293
2.4. NMR

Bruker Ultrashield spectrometer 400 MHz, solvent DMSO-d6, TMS standard. Concentration: 15 mg in 0.6 ml (Figs. 4–7).

Fig. 4. $^1$H NMR spectrum for 2-(1,3-oxazolin-2-yl)pyridine (Py-ox) in DMSO-d6.

Fig. 5. $^{13}$C NMR spectrum for 2-(1,3-oxazolin-2-yl)pyridine (Py-ox) in DMSO-d6.
2.5. GC–MS

Hewlett Packard HP7890 A GC system, equipped with 7000 GC/MS triple-quadrupol and HP-5 capilar 300 m × 0.32 mm column with 0.25 μm dimethylpolysiloxane stationary phase, dopped by 5% of phenylpolysiloxane (Figs. 8–11).

2.6. DSC

The melting temperatures were measured by differential scanning calorimetry DSC 2010 TA instrument calorimeter equipped with an automated sampler. The data were collected with the heat/cool/heat cycle at a heating rate of 10 °C/min under a nitrogen atmosphere (Figs. 12 and 13).
**Fig. 8.** GC analysis of 2-(1,3-oxazolin-2-yl)pyridine (Py-ox).

**Fig. 9.** MS analysis of 2-(1,3-oxazolin-2-yl)pyridine (Py-ox).
**Fig. 10.** GC analysis of 2,6-bis(1,3-oxazolin-2-yl)pyridine (Py-box).

**Fig. 11.** MS analysis of 2,6-bis(1,3-oxazolin-2-yl)pyridine (Py-box).
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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.09.129.
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