organic compounds

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

5-Iodo-3-phenyl-2,1-benzoxazole

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Received 2 February 2013; accepted 28 February 2013

Key indicators: single-crystal X-ray study; T = 100 K; mean σ (C–C) = 0.008 Å; R factor = 0.041; wR factor = 0.090; data-to-parameter ratio = 20.8.

The title compound, $C_{13}H_8INO$, was prepared by a condensation reaction of 4-nitrobenzene with phenylacetonitrile in NaOH–ethanol solution. There are two independent molecules in the asymmetric unit, in which the dihedral angles between the benzene ring and the benzoisoxazole unit are 4.2 (3) and 4.1 (3)°. The crystal packing is governed by C– $H \cdots N$, C– $I \cdots \pi$ and C– $I \cdots O$ interactions.

Related literature

For the biologial activity and applications of benzo[c]isoxazoles, see: McEvoy*et al.*(1968); Hester*et al.*(1989); Walsh*et al.*(1990); Angibaud*et al.*(2003). For a related structure, see:Teslenko*et al.*(2008). For a general synthetic procedure, see:Davis & Pizzini (1960).



Experimental

Crystal data $C_{13}H_81NO$ $M_r = 321.10$ Monoclinic, $P2_1$ a = 5.381 (3) Å b = 15.225 (7) Å c = 13.749 (7) Å $\beta = 94.92$ (3)°

| $V = 1122.2 (10) \text{ Å}^3$ |
|---|
| Z = 4 |
| Mo $K\alpha$ radiation |
| $\mu = 2.83 \text{ mm}^{-1}$ |
| T = 100 K |
| $0.25 \times 0.08 \times 0.03 \text{ mm}$ |



15060 measured reflections

 $R_{\rm int} = 0.053$

6015 independent reflections

4621 reflections with $I > 2\sigma(I)$

Data collection

Kuma KM-4-CCD four-circle diffractometer Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)

 $T_{\min} = 0.44, \ T_{\max} = 0.80$

Refinement

| $R[F^2 > 2\sigma(F^2)] = 0.041$ | H-atom parameters constrained |
|---------------------------------|--|
| $wR(F^2) = 0.090$ | $\Delta \rho_{\rm max} = 1.98 \ {\rm e} \ {\rm \AA}^{-3}$ |
| S = 1.00 | $\Delta \rho_{\rm min} = -1.01 \text{ e } \text{\AA}^{-3}$ |
| 6015 reflections | Absolute structure: Flack (1983), |
| 289 parameters | 1659 Friedel pairs |
| 1 restraint | Flack parameter: 0.00 (3) |

Table 1

Intermolecular interactions (Å, $^{\circ}$).

Cg is the centroid of the C1B-C6B ring.

| $D - H \cdot \cdot \cdot A$ | D-H | $H \cdots A$ | $D \cdots A$ | $D - \mathbf{H} \cdots A$ |
|---|------------------------|------------------------------|---------------------|---------------------------|
| $C3A - H3A \cdots N1B^{i}$ | 0.95 | 2.40 | 3.247 (7) | 149 |
| $C11A - H11A \cdots N1A^{n}$ | 0.95 | 2.47 | 3.339 (8) | 152 |
| $C4A = I1A \cdots Cg$ $C4B = I1B \cdots O1A$ | 2.100 (5) 2.100 (5) | 3.335(2) | 5.325 (7) | 150.0(2) 156.3(2) |
| Symmetry codes: (i) x, y, z | -1; (ii) $-x -$ | $1, y - \frac{1}{2}, -z + 1$ | ; (iii) $-x + 1, y$ | $-\frac{1}{2}, -z+1.$ |

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors are grateful to the State fund for fundamental research of Ukraine for the financial support (Project F54.3/004).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2554).

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supplementary materials

Acta Cryst. (2013). E69, o508 [doi:10.1107/S1600536813005862]

5-Iodo-3-phenyl-2,1-benzoxazole

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Comment

Our interest in benzo[c]isoxazoles is concerned with their application as precursors of a variety of bioactive compounds (Angibaud *et al.*, 2003; Walsh *et al.*, 1990; Hester *et al.*, 1989; McEvoy *et al.*, 1968). The title compound will be used in our further investigations as arylation agent in palladium-catalyzed reactions with alkenes and alkynes.

The title compound crystalizes in the noncentrosymmetric monoclinic $P2_1$ space group with two independent molecules in the asymmetric part (A and B), see Fig. 1. The molecules are almost planar, the dihedral angles between the mean planes of benzoisoxazole and benzene rings being 4.2 (3)° and 4.1 (3)° for A and B, respectively. The geometrical parameters of the molecules are similar and consistent with the previously studied 2,1-benzoxazole derivatives (Teslenko *et al.*, 2008).

Crystal packing is governed by hydrogen bonds of C–H···N type and other intermolecular interactions including C–I··· π and C–I···O. Intermolecular interactions C4A–I1A··· C_g^{iii} (C_g is a centroid of C1B/C6B aromatic ring) and C4B–I1B···O1A connect the molecules into chains propagating in *b*-axis direction along 2₁ screw axis (see Fig. 2). Hydrogen bond C3A–H3A···N1B^{*i*} connects the chains into corrugated layer parallel to the *bc*-plane. Hydrogen bond C11A–H11A···N1A^{*ii*} binds successive layers.

Experimental

Phenylacetonitrile (1.4 g, 12 mmol) and 5 ml of benzene solution of 4-iodonitrobenene (2.49 g, 10 mmol) were added with stirring to 40 ml of ethanol solution of potassium hydroxide (4 g, 0.1 mole). The mixture was stirred for 4 h at 323 K, then poured into 150 ml of water and acidified with hydrochloric acid. The precipitate was isolated by filtration, washed with water and dried. Recrystallization of crude product from ethanol gave 2.57 g (80% yield) of 5-iodo-3-phenyl-2,1-benzoxazole as pale yellow needles suitable for X-ray analysis, m.p. 390–391 K.

Refinement

All H atoms were found in difference Fourier maps. All H atoms were positioned geometrically and treated as riding on their carriers, with C–H = 0.95 Å and $U_{iso}(H)$ = values of $1.2U_{eq}(C)$.

Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).



Figure 1

The asymmetric unit of the title compound with atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level.



Figure 2

The crystal packing of the title compound showing intermolecular interactions as dashed lines (molecule A - red, molecule B - green).

5-Iodo-3-phenyl-2,1-benzoxazole

Crystal data

 $C_{13}H_8INO$ $M_r = 321.10$ Monoclinic, $P2_1$ Hall symbol: P 2yb a = 5.381 (3) Å b = 15.225 (7) Å c = 13.749 (7) Å $\beta = 94.92$ (3)° V = 1122.2 (10) Å³ Z = 4

Data collection

| Kuma KM-4-CCD four-circle |
|--|
| diffractometer |
| Radiation source: fine-focus sealed tube |
| Graphite monochromator |
| ω scans |
| Absorption correction: analytical |
| (CrysAlis RED; Oxford Diffraction, 2006) |
| $T_{\min} = 0.44, \ T_{\max} = 0.80$ |

Refinement

Refinement on F^2 Hydrogen site location: inferred from Least-squares matrix: full neighbouring sites $R[F^2 > 2\sigma(F^2)] = 0.041$ H-atom parameters constrained $wR(F^2) = 0.090$ $w = 1/[\sigma^2(F_o^2) + (0.046P)^2]$ where $P = (F_0^2 + 2F_c^2)/3$ S = 1.006015 reflections $(\Delta/\sigma)_{\rm max} = 0.001$ 289 parameters $\Delta \rho_{\rm max} = 1.98 \ {\rm e} \ {\rm \AA}^{-3}$ $\Delta \rho_{\rm min} = -1.01 \ e \ {\rm \AA}^{-3}$ 1 restraint Absolute structure: Flack (1983), 1659 Friedel Primary atom site location: structure-invariant direct methods pairs Flack parameter: 0.00 (3) Secondary atom site location: difference Fourier map

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.

F(000) = 616

 $\theta = 3.0 - 34.7^{\circ}$

 $\mu = 2.83 \text{ mm}^{-1}$

Needle, pale yellow

 $0.25\times0.08\times0.03~mm$

 $\theta_{\text{max}} = 34.7^{\circ}, \ \theta_{\text{min}} = 3.0^{\circ}$

15060 measured reflections 6015 independent reflections 4621 reflections with $I > 2\sigma(I)$

T = 100 K

 $R_{\rm int} = 0.053$

 $h = -8 \rightarrow 7$ $k = -17 \rightarrow 23$ $l = -20 \rightarrow 21$

 $D_{\rm x} = 1.901 {\rm Mg m^{-3}}$

Melting point = 390–391 K

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 15060 reflections

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 $(Å^2)$

| | x | У | Ζ | $U_{ m iso}$ */ $U_{ m eq}$ | |
|-----|-------------|-------------|-------------|-----------------------------|--|
| I1A | 0.51472 (6) | 0.01154 (2) | 0.19512 (2) | 0.02514 (9) | |
| O1A | -0.2353 (8) | 0.2574 (3) | 0.4305 (3) | 0.0262 (9) | |
| N1A | -0.0803 (9) | 0.3076 (4) | 0.3739 (4) | 0.0316 (10) | |

| C1A 0.0530 (10) 0.2453 (4) 0.322 (4) 0.0256 (12) C2A 0.2425 (11) 0.2666 (5) 0.0303 (13) H2A 0.2651 (11) 0.2002 (4) 0.2316 (4) 0.0261 (11) H3A 0.4926 0.2110 0.1894 0.031* C4A 0.3088 (10) 0.1115 (4) 0.2561 (4) 0.0219 (10) C5A 0.1314 (10) 0.0090 (4) 0.3171 (4) 0.0204 (10) C5A 0.0318 0.0309 0.3328 0.024* C6A -0.0029 (10) 0.1613 (3) 0.3564 (4) 0.0201 (10) C7A -0.1871 (10) 0.1707 (4) 0.4735 (4) 0.0260 (11) H9A -0.1608 -0.0034 0.4373 0.0267 (12) H10A -0.3325 (10) 0.0110 (4) 0.4735 (4) 0.0267 (12) H10A -0.3325 (10) 0.038 (4) 0.5750 (4) 0.0267 (12) H10A -0.6611 0.0883 (4) 0.5750 (4) 0.0229 (11) H11A -0.773 0.1054 0.6138 (0) < | | | | | |
|---|------|--------------|-------------|-------------|-------------|
| C2A 0.2425 (11) 0.2686 (4) 0.2666 (5) 0.0308 (13) H2A 0.2565 0.3276 0.2316 (4) 0.036* C3A 0.3651 (11) 0.2002 (4) 0.2316 (4) 0.0219 (10) H3A 0.4926 0.2110 0.1894 0.031* C4A 0.3088 (10) 0.1115 (4) 0.22561 (4) 0.0219 (10) C5A 0.1314 (10) 0.9030 (4) 0.3171 (4) 0.0204 (10) C5A 0.0391 (0) 0.1613 (3) 0.3564 (4) 0.0211 (10) C7A -0.1871 (10) 0.1707 (4) 0.4203 (4) 0.0220 (11) C9A -0.2385 (11) 0.0191 (4) 0.4735 (4) 0.0220 (11) H9A -0.1608 -0.0380 (4) 0.5730 (4) 0.0267 (12) H10A -0.3982 -0.0992 0.5230 0.032* C11A -0.6211 (10) -0.0438 (4) 0.5776 (4) 0.0229 (11) H1A -0.5707 0.2033 0.5300 0.027* C13A -0.6676 (11) 0.0838 (4) 0.5 | C1A | 0.0530 (10) | 0.2453 (4) | 0.3322 (4) | 0.0256 (12) |
| H2A 0.2765 0.3276 0.2499 0.036° C3A $0.3651(11)$ $0.2002(4)$ $0.2316(4)$ $0.0261(11)$ H3A 0.4926 0.2110 0.1894 0.031° C4A $0.3088(10)$ $0.1115(4)$ $0.2561(4)$ $0.0219(10)$ H5A 0.0981 0.0309 0.3328 0.024° C6A $-0.0029(10)$ $0.1613(3)$ $0.3564(4)$ $0.0201(10)$ C7A $-0.1871(10)$ $0.1707(4)$ $0.4203(4)$ $0.0213(10)$ C8A $-0.3335(10)$ $0.1101(4)$ $0.4735(4)$ $0.0204(10)$ C9A $-0.2895(11)$ $0.0191(4)$ $0.4735(4)$ $0.0260(11)$ H9A -0.1608 -0.0034 $0.5240(4)$ $0.02267(12)$ H10A -0.3982 -0.0992 0.5230 0.032° C11A $-0.6211(10)$ $-0.0980(4)$ $0.5750(4)$ $0.0229(11)$ H11A -0.7201 -0.0478 0.6084 0.036° C12A $-0.6676(11)$ $0.0838(4)$ $0.5776(4)$ $0.0229(1)$ H13A -0.5597 0.2033 0.5300 0.027° L13A -0.5597 0.2033 0.5300 0.027° L13A -0.5597 0.2033 0.5300 $0.0278(8)$ N1B $0.6242(9)$ $0.2244(3)$ $1.0482(4)$ $0.0270(10)$ C1B $0.4622(10)$ $0.2974(3)$ $0.9794(4)$ $0.0229(11)$ H13A -0.5597 $0.2353(3)$ $0.9704(4)$ $0.0220(11)$ H2B $0.2351(11)$ $0.3519(4)$ | C2A | 0.2425 (11) | 0.2686 (4) | 0.2666 (5) | 0.0303 (13) |
| C3A 0.3651 (11) 0.2002 (4) 0.2316 (4) 0.0211 (11) H3A 0.4926 0.2110 0.1894 0.031* C4A 0.3088 (10) 0.1115 (4) 0.22561 (4) 0.0219 (10) C5A 0.1314 (10) 0.0903 (4) 0.3171 (4) 0.0224* C6A -0.0029 (10) 0.1613 (3) 0.3564 (4) 0.0213 (10) C7A -0.1871 (10) 0.1707 (4) 0.4203 (4) 0.0220 (10) C8A -0.3335 (10) 0.1101 (4) 0.4753 (4) 0.0260 (11) H9A -0.1608 -0.0034 0.4373 0.031* C10A -0.4324 (12) -0.0380 (4) 0.5240 (4) 0.0267 (12) H1A -0.6211 (10) -0.0080 (4) 0.5750 (4) 0.0229 (11) H1A -0.7201 -0.0478 0.6084 0.36* C12A -0.6676 (11) 0.838 (4) 0.5776 (4) 0.0229 (11) H1A -0.7201 -0.0478 0.6084 0.36* C12A -0.6676 (11) 0.5828 (4) 0.0 | H2A | 0.2765 | 0.3276 | 0.2499 | 0.036* |
| H3A 0.4926 0.2110 0.1894 $0.031*$ C4A $0.3088 (10)$ $0.1115 (4)$ $0.2561 (4)$ $0.0219 (10)$ C5A $0.0314 (10)$ $0.0903 (4)$ $0.3171 (4)$ $0.0204 (10)$ H5A 0.0981 0.3030 0.3328 $0.024*$ C6A $-0.0029 (10)$ $0.1613 (3)$ $0.3564 (4)$ $0.0201 (10)$ C7A $-0.1871 (10)$ $0.1707 (4)$ $0.4203 (4)$ $0.0213 (10)$ C8A $-0.3335 (10)$ $0.1101 (4)$ $0.4753 (4)$ $0.0260 (11)$ H9A -0.1688 -0.0034 0.4373 $0.031*$ C10A $-0.4324 (12)$ $-0.0380 (4)$ $0.5750 (4)$ $0.0260 (12)$ H10A $-0.2985 (1)$ -0.0992 0.5230 $0.032*$ C11A $-0.6211 (10)$ -0.0992 0.5230 $0.032*$ C11A $-0.676 (11)$ $0.0838 (4)$ $0.5776 (4)$ $0.0229 (11)$ H12A -0.7973 0.1054 0.6188 $0.027*$ C13A $-0.5264 (10)$ $0.1421 (4)$ $0.5282 (4)$ $0.0220 (1)$ H13A -0.597 0.2033 0.5300 $0.026*$ HB $-0.05111 (7)$ $0.30782 (2)$ $0.66188 (3)$ $0.0271 (9)$ OHB $0.542 (9)$ $0.2347 (3)$ $0.9704 (4)$ $0.0232 (11)$ C1B $0.4622 (10)$ $0.2937 (3)$ $0.9704 (4)$ $0.0232 (11)$ C1B $0.4622 (10)$ $0.2381 (3)$ $0.9704 (4)$ $0.0232 (11)$ C1B $0.216 (1)$ $0.2353 (3)$ $0.9704 (4)$ $0.0226 (10)$ <td>C3A</td> <td>0.3651 (11)</td> <td>0.2002 (4)</td> <td>0.2316 (4)</td> <td>0.0261 (11)</td> | C3A | 0.3651 (11) | 0.2002 (4) | 0.2316 (4) | 0.0261 (11) |
| C4A0.3088 (10)0.1115 (4)0.2561 (4)0.0219 (10)C5A0.1314 (10)0.0903 (4)0.3171 (4)0.0204 (10)L5A0.0029 (10)0.1613 (3)0.3564 (4)0.0211 (10)C7A-0.1871 (10)0.1707 (4)0.4203 (4)0.0213 (10)C8A-0.3335 (10)0.1101 (4)0.4755 (4)0.0206 (11)L9A-0.2895 (11)0.0191 (4)0.4755 (4)0.0206 (11)L9A-0.1608-0.00340.43730.031*C10A-0.4324 (12)-0.0380 (4)0.5240 (4)0.0267 (12)H10A-0.3982-0.09920.52300.032*C11A-0.6211 (10)-0.0080 (4)0.5750 (4)0.0229 (11)H11A-0.7201-0.04780.60840.36*C12A-0.6676 (11)0.0838 (4)0.5776 (4)0.0229 (11)H12A-0.79730.10540.61380.027*C13A-0.55970.20330.53000.026*H1B-0.05111 (7)0.30782 (2)0.6158 (3)0.0271 (9)O1B0.7816 (8)0.2167 (3)1.0422 (4)0.0270 (10)C1B0.4622 (9)0.2344 (3)1.0482 (4)0.0270 (10)C1B0.45790.2974 (3)0.7956 (4)0.0244 (11)C1B0.1261 (11)0.3519 (4)0.9904 (11)C1B0.452 (9)0.2344 (4)0.0270 (10)C1B0.4622 (10)0.2974 (3)0.7956 (4)0.0206 (10)C1B0.4579 (9)0.2374 (4)0.8739 (4) <td>H3A</td> <td>0.4926</td> <td>0.2110</td> <td>0.1894</td> <td>0.031*</td> | H3A | 0.4926 | 0.2110 | 0.1894 | 0.031* |
| C5A 0.1314 (10) 0.0003 (4) 0.3171 (4) 0.0204 (10) H5A 0.0981 0.0309 0.3328 0.024* C6A -0.0029 (10) 0.1613 (3) 0.3564 (4) 0.0213 (10) C7A -0.1871 (10) 0.1707 (4) 0.4203 (4) 0.0213 (10) C8A -0.3335 (10) 0.1101 (4) 0.4753 (4) 0.0206 (11) H9A -0.1608 -0.0034 0.4373 0.031* C10A -0.4324 (12) -0.0380 (4) 0.5240 (4) 0.0267 (12) H10A -0.7201 -0.0478 0.6084 0.036* C12A -0.6676 (11) 0.838 (4) 0.5776 (4) 0.0229 (11) H1A -0.7201 -0.0478 0.6138 0.027* C13A -0.5264 (10) 0.1421 (4) 0.5282 (4) 0.0220 (11) H13A -0.5597 0.2033 0.5300 0.026* HB -0.0511 (7) 0.30782 (2) 0.66158 (3) 0.0271 (19) O1B 0.7816 (8) 0.2167 (3) 1.0422 (3) | C4A | 0.3088 (10) | 0.1115 (4) | 0.2561 (4) | 0.0219 (10) |
| H5A 0.0981 0.0390 0.3328 0.024^* C6A $-0.0029(10)$ $0.1613(3)$ $0.3564(4)$ $0.0201(10)$ C7A $-0.1871(10)$ $0.1707(4)$ $0.4203(4)$ $0.0213(10)$ C8A $-0.3335(10)$ $0.1101(4)$ $0.4753(4)$ $0.0204(10)$ C9A $-0.2895(11)$ $0.0191(4)$ $0.4735(4)$ $0.0204(10)$ C10A $-0.4324(12)$ -0.0034 $0.4735(4)$ $0.0267(12)$ H10A -0.3982 -0.0992 0.5230 0.032^* C11A $-0.6211(10)$ $-0.0080(4)$ $0.5750(4)$ $0.2296(14)$ H11A -0.7201 -0.0478 0.6084 $0.0267(12)$ H12A $-0.6676(11)$ $0.0838(4)$ $0.5776(4)$ $0.0229(11)$ H12A $-0.5264(10)$ $0.1421(4)$ $0.5282(4)$ $0.0220(11)$ H13A -0.5597 0.2033 0.5300 0.027^* C13A $-0.5264(10)$ $0.1421(4)$ $0.5282(4)$ $0.0270(10)$ H1B $-0.511(7)$ $0.30782(2)$ $0.66158(3)$ $0.02711(9)$ O1B $0.7816(8)$ $0.2167(3)$ $1.0229(3)$ $0.2258(8)$ N1B $0.6242(9)$ $0.2844(3)$ $1.0482(4)$ $0.270(10)$ C1B $0.4522(10)$ $0.2397(3)$ $0.9704(4)$ $0.2329(11)$ C1B $0.3590(1)$ $0.3530(4)$ $0.0249(1)$ H3B -0.0353 0.3907 0.8673 0.030^* C1B $0.157(9)$ $0.2384(4)$ $0.756(4)$ $0.2020(1)$ C1B $0.3599(10)$ 0.23 | C5A | 0.1314 (10) | 0.0903 (4) | 0.3171 (4) | 0.0204 (10) |
| C6A -0.0029 (10) 0.1613 (3) 0.3564 (4) 0.0210 (10) C7A -0.1871 (10) 0.1707 (4) 0.4203 (4) 0.0213 (10) C8A -0.3355 (10) 0.1101 (4) 0.4735 (4) 0.0204 (10) C9A -0.2895 (11) 0.0191 (4) 0.4735 (4) 0.0260 (11) H9A -0.1608 -0.0034 0.4373 0.031* C10A -0.6211 (10) -0.0380 (4) 0.5240 (4) 0.0267 (12) H10A -0.388 (2) -0.0992 0.5230 0.032* C12A -0.6676 (11) 0.0838 (4) 0.5776 (4) 0.0229 (11) H12A -0.7973 0.1054 0.6138 0.027* C13A -0.5264 (10) 0.1421 (4) 0.5282 (4) 0.0220 (11) H13A -0.5577 0.2033 0.5300 0.026* H1B -0.05111 (7) 0.30782 (2) 0.66158 (3) 0.02711 (9) O1B 0.7816 (8) 0.2167 (3) 1.0229 (3) 0.0284 (8) C1B 0.6242 (9) 0.2844 (3) | H5A | 0.0981 | 0.0309 | 0.3328 | 0.024* |
| C7A $-0.1871 (10)$ $0.1707 (4)$ $0.4203 (4)$ $0.0213 (10)$ $C8A$ $-0.3335 (10)$ $0.1101 (4)$ $0.4735 (4)$ $0.0204 (10)$ $C9A$ $-0.2895 (11)$ $0.0191 (4)$ $0.4735 (4)$ $0.0260 (11)$ $H9A$ -0.1608 -0.034 0.4373 $0.031*$ $C10A$ $-0.4324 (12)$ $-0.0380 (4)$ $0.5240 (4)$ $0.0267 (12)$ $H10A$ -0.3982 -0.0992 0.5230 $0.032*$ $C11A$ $-0.6671 (10)$ $-0.0080 (4)$ $0.5750 (4)$ $0.0296 (14)$ $H1A$ -0.7201 -0.0478 0.6084 $0.036*$ $C12A$ $-0.6676 (11)$ $0.0838 (4)$ $0.5776 (4)$ $0.0229 (11)$ $H1A$ $-0.5264 (10)$ $0.1421 (4)$ $0.5282 (4)$ $0.0220 (11)$ $H1A$ -0.5597 0.2033 0.5300 $0.027*$ $C13A$ -0.5597 0.2033 0.5300 $0.0278 (8)$ $N1B$ $0.6242 (9)$ $0.2844 (3)$ $1.0482 (4)$ $0.0270 (10)$ $C1B$ $0.4622 (10)$ $0.237 (3)$ $0.9704 (4)$ $0.0232 (11)$ $C1B$ $0.4622 (10)$ $0.2397 (3)$ $0.9704 (4)$ $0.0249 (11)$ $H3B$ -0.0335 0.3907 0.8673 $0.030*$ $C4B$ $0.1074 (11)$ $0.3530 (4)$ $0.0226 (10)$ $C13B$ 0.3902 0.2010 $0.751 (0.026* (10)$ $C13B$ 0.3902 $0.2914 (3)$ $0.795 (4)$ $0.0226 (10)$ $C1B$ $0.3519 (10)$ $0.187 (3)$ $0.9304 (4)$ $0.0220 (11)$ | C6A | -0.0029 (10) | 0.1613 (3) | 0.3564 (4) | 0.0201 (10) |
| C8A -0.3355 (10) 0.1101 (4) 0.4735 (4) 0.0204 (10) C9A -0.2895 (11) 0.0191 (4) 0.4735 (4) 0.0260 (11) H9A -0.1608 -0.034 0.4373 0.031* C10A -0.4324 (12) -0.0380 (4) 0.5240 (4) 0.0267 (12) H10A -0.3982 -0.0992 0.5230 0.032* C11A -0.6211 (10) -0.0080 (4) 0.5750 (4) 0.0229 (14) H11A -0.7201 -0.0478 0.6084 0.032* C13A -0.6676 (11) 0.0388 (4) 0.5776 (4) 0.0229 (11) H12A -0.7973 0.1054 0.6138 0.0227 (11) H13A -0.5597 0.2033 0.5300 0.026* H1B -0.05111 (7) 0.30782 (2) 0.66158 (3) 0.0271 (10) O1B 0.7816 (8) 0.2167 (3) 1.0422 (4) 0.0270 (10) C1B 0.4622 (10) 0.2397 (3) 0.9704 (4) 0.0232 (11) C2B 0.25131 (11) 0.3519 (4) 0.92 | C7A | -0.1871 (10) | 0.1707 (4) | 0.4203 (4) | 0.0213 (10) |
| C9A -0.2895 (11) 0.0191 (4) 0.4735 (4) 0.0260 (11) H9A -0.1608 -0.0034 0.4373 0.031* C10A -0.4324 (12) -0.0380 (4) 0.5240 (4) 0.0267 (12) H10A -0.0211 (10) -0.0080 (4) 0.5750 (4) 0.0226 (14) H11A -0.6211 (10) -0.0478 0.6084 0.036* C12A -0.6676 (11) 0.0838 (4) 0.5776 (4) 0.0229 (11) H12A -0.5264 (10) 0.1421 (4) 0.5282 (4) 0.0220 (11) H13A -0.5597 0.2033 0.5300 0.026* H1B -0.05111 (7) 0.30782 (2) 0.66158 (3) 0.02711 (9) O1B 0.7816 (8) 0.2167 (3) 1.0229 (3) 0.0258 (8) N1B 0.6242 (9) 0.2844 (3) 1.0482 (4) 0.0232 (11) C2B 0.2531 (11) 0.3519 (4) 0.9704 (4) 0.0232 (11) C2B 0.2531 (11) 0.3530 (4) 0.0249 (11) M3B -0.0353 0.3907 0.8673 <td>C8A</td> <td>-0.3335 (10)</td> <td>0.1101 (4)</td> <td>0.4753 (4)</td> <td>0.0204 (10)</td> | C8A | -0.3335 (10) | 0.1101 (4) | 0.4753 (4) | 0.0204 (10) |
| H9A-0.1608-0.00340.43730.031*C10A-0.4324 (12)-0.0380 (4)0.5240 (4)0.0267 (12)H10A-0.3982-0.09920.52300.032*C11A-0.6211 (10)-0.0080 (4)0.5750 (4)0.0296 (14)H11A-0.7201-0.04780.60840.036*C12A-0.6676 (11)0.0838 (4)0.5776 (4)0.0229 (11)H12A-0.79730.10540.61380.022*C13A-0.5264 (10)0.1421 (4)0.5282 (4)0.0220 (11)H13A-0.55970.20330.53000.026*11B-0.05111 (7)0.30782 (2)0.66158 (3)0.02711 (9)01B0.7816 (8)0.2167 (3)1.0229 (3)0.0258 (8)N1B0.6242 (9)0.2844 (3)1.0482 (4)0.0270 (10)C1B0.4622 (10)0.2937 (3)0.9704 (4)0.0222 (11)C2B0.2531 (11)0.3519 (4)0.9611 (5)0.0272 (12)H2B0.21660.38901.01360.033*C3B0.1074 (11)0.3530 (4)0.8749 (4)0.0226 (10)C5B0.3589 (10)0.2384 (4)0.8030 (4)0.0226 (11)H3B-0.0350.39070.86730.030*C4B0.157 (9)0.2974 (3)0.956 (4)0.0226 (12)C5B0.3589 (10)0.2384 (4)0.8030 (4)0.0196 (10)C5B0.3589 (10)0.2383 (3)0.8931 (4)0.0196 (10)C6B0.5112 (10)0.2353 (3)0.8959 | C9A | -0.2895 (11) | 0.0191 (4) | 0.4735 (4) | 0.0260 (11) |
| C10A -0.4324 (12) -0.0380 (4) 0.5240 (4) 0.0267 (12)H10A -0.3982 -0.0992 0.5230 $0.032*$ C11A -0.6211 (10) -0.0080 (4) 0.5750 (4) 0.0296 (14)H11A -0.7201 -0.0478 0.6084 $0.036*$ C12A -0.6676 (1) 0.0838 (4) 0.5776 (4) 0.0229 (1)H12A -0.7973 0.1054 0.5138 $0.027*$ C13A -0.5597 0.2033 0.5300 $0.026*$ HB -0.05111 (7) 0.30782 (2) 0.66158 (3) 0.02711 (9)O1B 0.7816 (8) 0.2167 (3) 1.0229 (3) 0.0258 (8)NIB 0.6242 (9) 0.2844 (3) 1.0482 (4) 0.0270 (10)C1B 0.4622 (10) 0.2937 (3) 0.9704 (4) 0.0222 (11)C2B 0.2531 (11) 0.3519 (4) 0.9611 (5) 0.0272 (12)H2B 0.2166 0.3890 1.0136 $0.033*$ C3B 0.1074 (11) 0.3530 (4) 0.8673 $0.300*$ C4B 0.1657 (9) 0.2974 (3) 0.7956 (4) 0.0226 (10)C5B 0.3589 (10) 0.2384 (4) 0.8030 (4) 0.0199 (10)C7B 0.5112 (10) 0.2353 (3) 0.8931 (4) 0.0196 (10)C8B 0.8618 (10) 0.1135 (4) 0.8931 (4) 0.0226 (12)C1B 0.5182 (12) 0.0214 0.0225 (12)H9B 0.6644 0.0996 0.7621 $0.031*$ C1BB 0.9 | H9A | -0.1608 | -0.0034 | 0.4373 | 0.031* |
| H10A-0.3982-0.09920.52300.032*C11A-0.6211 (10)-0.0080 (4)0.5750 (4)0.0296 (14)H11A-0.7201-0.04780.60840.036*C12A-0.6676 (11)0.0838 (4)0.5776 (4)0.0229 (11)H12A-0.79730.10540.61380.027*C13A-0.5264 (10)0.1421 (4)0.5282 (4)0.0220 (11)H13A-0.55970.20330.53000.026*IB-0.05111 (7)0.30782 (2)0.66158 (3)0.02711 (9)O1B0.7816 (8)0.2167 (3)1.0229 (3)0.0258 (8)N1B0.6242 (9)0.2844 (3)1.0482 (4)0.0270 (10)C1B0.4622 (10)0.2937 (3)0.9704 (4)0.0222 (11)C2B0.2531 (11)0.3519 (4)0.9611 (5)0.0272 (12)H2B0.21660.38901.01360.033*C3B0.1074 (11)0.3530 (4)0.8749 (4)0.0249 (11)H3B-0.03350.39070.86730.030*C4B0.157 (9)0.2974 (3)0.7956 (4)0.0220 (11)H5B0.39020.20100.75010.026*C6B0.5112 (10)0.2353 (3)0.8931 (4)0.0199 (10)C7B0.7150 (10)0.1375 (4)0.8959 (4)0.0216 (10)C7B0.9389 (10)0.082 (4)0.7220 (4)0.0258 (12)H9B0.66440.09960.76210.031*C10B0.9389 (10)0.082 (4)0.72890.031* <td>C10A</td> <td>-0.4324 (12)</td> <td>-0.0380 (4)</td> <td>0.5240 (4)</td> <td>0.0267 (12)</td> | C10A | -0.4324 (12) | -0.0380 (4) | 0.5240 (4) | 0.0267 (12) |
| C11A $-0.6211 (10)$ $-0.0080 (4)$ $0.5750 (4)$ $0.0296 (14)$ H11A -0.7201 -0.0478 0.6084 $0.036*$ C12A $-0.6676 (11)$ $0.0838 (4)$ $0.5776 (4)$ $0.0229 (11)$ H12A -0.7973 0.1054 0.6138 $0.027*$ C13A $-0.5264 (10)$ $0.1421 (4)$ $0.5282 (4)$ $0.0220 (11)$ H13A -0.5597 0.2033 0.5300 $0.026*$ IB $-0.05111 (7)$ $0.30782 (2)$ $0.66158 (3)$ $0.0271 (9)$ O1B $0.7816 (8)$ $0.2167 (3)$ $1.0229 (3)$ $0.0258 (8)$ N1B $6.6242 (9)$ $0.2844 (3)$ $1.0482 (4)$ $0.0270 (10)$ C1B $0.4622 (10)$ $0.2937 (3)$ $0.9704 (4)$ $0.0222 (11)$ C2B $0.2531 (11)$ $0.3519 (4)$ $0.9611 (5)$ $0.0272 (12)$ H2B 0.2166 0.3890 1.0136 $0.033*$ C3B $0.1074 (11)$ $0.3530 (4)$ 0.8737 0.304^* C4B $0.1657 (9)$ $0.2974 (3)$ $0.7956 (4)$ $0.0206 (10)$ C5B $0.3589 (10)$ $0.238 (4)$ $0.8030 (4)$ $0.0220 (11)$ H5B 0.3902 0.2010 0.7501 $0.026*$ C6B $0.5112 (10)$ $0.2353 (3)$ $0.8931 (4)$ $0.0196 (10)$ C7B $0.8005 (11)$ $0.706 (4)$ $0.8031 (4)$ $0.0258 (12)$ H9B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389 (10)$ $0.0082 (4)$ $0.7720 (4)$ $0.0255 (10)$ <tr< td=""><td>H10A</td><td>-0.3982</td><td>-0.0992</td><td>0.5230</td><td>0.032*</td></tr<> | H10A | -0.3982 | -0.0992 | 0.5230 | 0.032* |
| H11A -0.7201 -0.0478 0.6084 $0.036*$ C12A $-0.6676 (11)$ $0.0838 (4)$ $0.5776 (4)$ $0.0229 (11)$ H12A -0.7973 0.1054 0.6138 $0.027*$ C13A -0.5597 0.2033 0.5300 $0.026*$ HB $-0.05111 (7)$ $0.30782 (2)$ $0.66158 (3)$ $0.02711 (9)$ O1B $0.7816 (8)$ $0.2167 (3)$ $1.0229 (3)$ $0.0258 (8)$ N1B $0.6242 (9)$ $0.2844 (3)$ $1.0482 (4)$ $0.0270 (10)$ C1B $0.4622 (10)$ $0.2937 (3)$ $0.9704 (4)$ $0.0232 (11)$ C2B $0.2531 (11)$ $0.3519 (4)$ $0.9611 (5)$ $0.0272 (12)$ H2B 0.2166 0.3890 1.0136 $0.033*$ C3B $0.1074 (11)$ $0.3530 (4)$ $0.8749 (4)$ $0.0249 (11)$ H3B -0.0335 0.3907 0.8673 $0.300*$ C4B $0.1657 (9)$ $0.2974 (3)$ $0.7956 (4)$ $0.0226 (10)$ C5B $0.3589 (10)$ $0.2384 (4)$ $0.8030 (4)$ $0.0220 (11)$ H5B 0.3902 0.2010 0.7501 $0.026*$ C6B $0.5112 (10)$ $0.2353 (3)$ $0.8931 (4)$ $0.0199 (10)$ C7B $0.3989 (10)$ $0.1873 (3)$ $0.9304 (4)$ $0.0196 (10)$ C7B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389 (10)$ $0.082 (4)$ $0.7720 (4)$ $0.0225 (10)$ H10B $1.323 (12)$ -0.0753 0.8076 $0.034*$ C10B 0.938 | C11A | -0.6211 (10) | -0.0080 (4) | 0.5750 (4) | 0.0296 (14) |
| C12A -0.6676 (11) 0.0838 (4) 0.5776 (4) 0.0229 (11) H12A -0.7973 0.1054 0.6138 0.027* C13A -0.5264 (10) 0.1421 (4) 0.5282 (4) 0.0220 (11) H13A -0.5597 0.2033 0.5300 0.026* IIB -0.05111 (7) 0.30782 (2) 0.66158 (3) 0.02711 (9) O1B 0.7816 (8) 0.2167 (3) 1.0229 (3) 0.0258 (8) NIB 0.6242 (9) 0.2844 (3) 1.0482 (4) 0.0270 (10) C1B 0.4622 (10) 0.2937 (3) 0.9704 (4) 0.0222 (11) C2B 0.2531 (11) 0.3519 (4) 0.9611 (5) 0.0272 (12) H2B 0.166 0.3890 1.0136 0.033* C3B 0.1074 (11) 0.3530 (4) 0.8749 (4) 0.0206 (10) C5B 0.3589 (10) 0.2384 (4) 0.8030 (4) 0.0206 (10) C5B 0.5112 (10) 0.2353 (3) 0.8931 (4) 0.0199 (10) C7B 0.7150 (10 0.1873 (3) | H11A | -0.7201 | -0.0478 | 0.6084 | 0.036* |
| H12A-0.79730.10540.61380.027*C13A-0.5264 (10)0.1421 (4)0.5282 (4)0.0220 (11)H13A-0.55970.20330.53000.026*IB-0.05111 (7)0.30782 (2)0.66158 (3)0.02711 (9)O1B0.7816 (8)0.2167 (3)1.0229 (3)0.0258 (8)N1B0.6242 (9)0.2844 (3)1.0482 (4)0.0270 (10)C1B0.4622 (10)0.2937 (3)0.9704 (4)0.0232 (11)C2B0.2531 (11)0.3519 (4)0.9611 (5)0.0272 (12)H2B0.21660.38901.01360.033*C3B0.1074 (11)0.3530 (4)0.8749 (4)0.0249 (11)H3B-0.03350.39070.86730.300*C4B0.1657 (9)0.2974 (3)0.7956 (4)0.0206 (10)C5B0.3589 (10)0.2383 (3)0.8030 (4)0.0199 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C8B0.8618 (10)0.1135 (4)0.8959 (4)0.0216 (10)C9B0.8005 (11)0.0769 (4)0.8031 (4)0.0255 (10)H10B0.8969-0.01580.70890.031*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96 | C12A | -0.6676 (11) | 0.0838 (4) | 0.5776 (4) | 0.0229 (11) |
| C13A -0.5264 (10) 0.1421 (4) 0.5282 (4) 0.0220 (11) H13A -0.5597 0.2033 0.5300 0.026* I1B -0.05111 (7) 0.30782 (2) 0.66158 (3) 0.02711 (9) O1B 0.7816 (8) 0.2167 (3) 1.0229 (3) 0.0258 (8) N1B 0.6242 (9) 0.2844 (3) 1.0482 (4) 0.0270 (10) C1B 0.4622 (10) 0.2937 (3) 0.9704 (4) 0.0229 (11) C2B 0.2531 (11) 0.3519 (4) 0.9611 (5) 0.0224 (11) C3B 0.1074 (11) 0.3530 (4) 0.8749 (4) 0.0249 (11) H3B -0.0335 0.3907 0.8673 0.030* C4B 0.1657 (9) 0.2974 (3) 0.7956 (4) 0.0206 (10) C5B 0.3589 (10) 0.2384 (4) 0.8030 (4) 0.0220 (11) H5B 0.3902 0.2010 0.7501 0.026* C6B 0.5112 (10) 0.2353 (3) 0.8931 (4) 0.0199 (10) C7B 0.7150 (10) 0.1873 (3) | H12A | -0.7973 | 0.1054 | 0.6138 | 0.027* |
| H13A-0.55970.20330.53000.026*IIB-0.05111 (7)0.30782 (2)0.66158 (3)0.02711 (9)O1B0.7816 (8)0.2167 (3)1.0229 (3)0.0258 (8)N1B0.6242 (9)0.2844 (3)1.0482 (4)0.0270 (10)C1B0.4622 (10)0.2937 (3)0.9704 (4)0.0232 (11)C2B0.2531 (11)0.3519 (4)0.9611 (5)0.0272 (12)H2B0.21660.38901.01360.033*C3B0.1074 (11)0.3530 (4)0.8749 (4)0.0249 (11)H3B-0.03350.39070.86730.030*C4B0.1657 (9)0.2974 (3)0.7956 (4)0.0206 (10)C5B0.3589 (10)0.2384 (4)0.8030 (4)0.0220 (11)H5B0.39020.20100.75010.026*C6B0.5112 (10)0.2353 (3)0.8931 (4)0.0199 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C8B0.8618 (10)0.1135 (4)0.8959 (4)0.0216 (10)C9B0.8005 (11)0.0769 (4)0.8031 (4)0.0258 (12)H9B0.66440.09960.76210.031*C10B0.9389 (10)0.0082 (4)0.7720 (4)0.0228 (12)H10B0.8969-0.01580.80760.034*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80660.034*C12B1.1968 (11)0.0999 (5)0.9218 (4)< | C13A | -0.5264 (10) | 0.1421 (4) | 0.5282 (4) | 0.0220 (11) |
| IIB -0.05111 (7) 0.30782 (2) 0.66158 (3) 0.02711 (9) OIB 0.7816 (8) 0.2167 (3) 1.0229 (3) 0.0258 (8) NIB 0.6242 (9) 0.2844 (3) 1.0482 (4) 0.0270 (10) CIB 0.4622 (10) 0.2937 (3) 0.9704 (4) 0.0232 (11) C2B 0.2531 (11) 0.3519 (4) 0.9611 (5) 0.0272 (12) H2B 0.2166 0.3890 1.0136 0.033* C3B 0.1074 (11) 0.3530 (4) 0.8749 (4) 0.0249 (11) H3B -0.0335 0.3907 0.8673 0.030* C4B 0.1657 (9) 0.2974 (3) 0.7956 (4) 0.0220 (11) H5B 0.3902 0.2010 0.7501 0.026* C6B 0.5112 (10) 0.2353 (3) 0.8931 (4) 0.0196 (10) C7B 0.7150 (10) 0.1873 (3) 0.9304 (4) 0.0196 (10) C8B 0.8005 (11) 0.0769 (4) 0.8031 (4) 0.0216 (10) C9B 0.8005 (11) 0.0769 (4) < | H13A | -0.5597 | 0.2033 | 0.5300 | 0.026* |
| O1B0.7816 (8)0.2167 (3)1.0229 (3)0.0258 (8)N1B0.6242 (9)0.2844 (3)1.0482 (4)0.0270 (10)C1B0.4622 (10)0.2937 (3)0.9704 (4)0.0232 (11)C2B0.2531 (11)0.3519 (4)0.9611 (5)0.0272 (12)H2B0.21660.38901.01360.033*C3B0.1074 (11)0.3530 (4)0.8749 (4)0.0249 (11)H3B-0.03350.39070.86730.030*C4B0.1657 (9)0.2974 (3)0.7956 (4)0.0206 (10)C5B0.3589 (10)0.2384 (4)0.8030 (4)0.0220 (11)H5B0.39020.20100.75010.026*C6B0.5112 (10)0.2353 (3)0.8931 (4)0.0199 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C8B0.8618 (10)0.1135 (4)0.8959 (4)0.0216 (10)C9B0.8005 (11)0.0769 (4)0.8031 (4)0.0258 (12)H9B0.66440.09960.76210.031*C10B0.9389 (10)0.0082 (4)0.7720 (4)0.0255 (10)H10B0.8969-0.01580.70890.031*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4) | I1B | -0.05111 (7) | 0.30782 (2) | 0.66158 (3) | 0.02711 (9) |
| N1B0.6242 (9)0.2844 (3)1.0482 (4)0.0270 (10)C1B0.4622 (10)0.2937 (3)0.9704 (4)0.0232 (11)C2B0.2531 (11)0.3519 (4)0.9611 (5)0.0272 (12)H2B0.21660.38901.01360.033*C3B0.1074 (11)0.3530 (4)0.8749 (4)0.0249 (11)H3B-0.03350.39070.86730.030*C4B0.1657 (9)0.2974 (3)0.7956 (4)0.0220 (10)C5B0.3589 (10)0.2384 (4)0.8030 (4)0.0220 (11)H5B0.39020.20100.75010.026*C6B0.5112 (10)0.2353 (3)0.8931 (4)0.0199 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C8B0.8618 (10)0.1135 (4)0.8959 (4)0.0216 (10)C9B0.8005 (11)0.0769 (4)0.8031 (4)0.0258 (12)H9B0.66440.09960.76210.031*C10B0.9389 (10)0.0082 (4)0.7720 (4)0.0255 (10)H10B0.8969-0.01580.70890.031*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.30* <td>O1B</td> <td>0.7816 (8)</td> <td>0.2167 (3)</td> <td>1.0229 (3)</td> <td>0.0258 (8)</td> | O1B | 0.7816 (8) | 0.2167 (3) | 1.0229 (3) | 0.0258 (8) |
| C1B $0.4622 (10)$ $0.2937 (3)$ $0.9704 (4)$ $0.0232 (11)$ C2B $0.2531 (11)$ $0.3519 (4)$ $0.9611 (5)$ $0.0272 (12)$ H2B 0.2166 0.3890 1.0136 $0.033*$ C3B $0.1074 (11)$ $0.3530 (4)$ $0.8749 (4)$ $0.0249 (11)$ H3B -0.0335 0.3907 0.8673 $0.030*$ C4B $0.1657 (9)$ $0.2974 (3)$ $0.7956 (4)$ $0.0206 (10)$ C5B $0.3589 (10)$ $0.2384 (4)$ $0.8030 (4)$ $0.0220 (11)$ H5B 0.3902 0.2010 0.7501 $0.026*$ C6B $0.5112 (10)$ $0.2353 (3)$ $0.9931 (4)$ $0.0199 (10)$ C7B $0.7150 (10)$ $0.1135 (4)$ $0.8959 (4)$ $0.0216 (10)$ C8B $0.8618 (10)$ $0.1135 (4)$ $0.8959 (4)$ $0.0216 (10)$ C9B $0.8005 (11)$ $0.0769 (4)$ $0.8031 (4)$ $0.0258 (12)$ H9B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389 (10)$ $0.0082 (4)$ $0.7720 (4)$ $0.0255 (10)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383 (12)$ $-0.0274 (4)$ $0.8297 (4)$ $0.0225 (12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968 (11)$ $0.0099 (5)$ $0.9218 (4)$ $0.0301 (11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630 (11)$ $0.0790 (4)$ $0.9549 (4)$ $0.0253 (11)$ <td>N1B</td> <td>0.6242 (9)</td> <td>0.2844 (3)</td> <td>1.0482 (4)</td> <td>0.0270 (10)</td> | N1B | 0.6242 (9) | 0.2844 (3) | 1.0482 (4) | 0.0270 (10) |
| C2B $0.2531 (11)$ $0.3519 (4)$ $0.9611 (5)$ $0.0272 (12)$ H2B 0.2166 0.3890 1.0136 $0.033*$ C3B $0.1074 (11)$ $0.3530 (4)$ $0.8749 (4)$ $0.0249 (11)$ H3B -0.0335 0.3907 0.8673 $0.030*$ C4B $0.1657 (9)$ $0.2974 (3)$ $0.7956 (4)$ $0.0220 (10)$ C5B $0.3589 (10)$ $0.2384 (4)$ $0.8030 (4)$ $0.0220 (11)$ H5B 0.3902 0.2010 0.7501 $0.026*$ C6B $0.5112 (10)$ $0.2353 (3)$ $0.8931 (4)$ $0.0199 (10)$ C7B $0.7150 (10)$ $0.1135 (4)$ $0.8959 (4)$ $0.0216 (10)$ C8B $0.8618 (10)$ $0.1135 (4)$ $0.8959 (4)$ $0.0226 (12)$ C10B $0.9389 (10)$ $0.0082 (4)$ $0.7720 (4)$ $0.0255 (12)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383 (12)$ $-0.0274 (4)$ $0.8297 (4)$ $0.0285 (12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968 (11)$ $0.0099 (5)$ $0.9218 (4)$ $0.0301 (11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630 (11)$ $0.0790 (4)$ $0.9549 (4)$ $0.0253 (11)$ | C1B | 0.4622 (10) | 0.2937 (3) | 0.9704 (4) | 0.0232 (11) |
| H2B0.21660.38901.01360.033*C3B0.1074 (11)0.3530 (4)0.8749 (4)0.0249 (11)H3B-0.03350.39070.86730.030*C4B0.1657 (9)0.2974 (3)0.7956 (4)0.0206 (10)C5B0.3589 (10)0.2384 (4)0.8030 (4)0.0220 (11)H5B0.39020.20100.75010.026*C6B0.5112 (10)0.2353 (3)0.8931 (4)0.0199 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C8B0.8618 (10)0.1135 (4)0.8959 (4)0.0216 (10)C9B0.8005 (11)0.0769 (4)0.8031 (4)0.0258 (12)H9B0.66440.09960.76210.031*C10B0.9389 (10)0.0082 (4)0.7720 (4)0.0255 (10)H10B0.8969-0.01580.70890.031*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | C2B | 0.2531 (11) | 0.3519 (4) | 0.9611 (5) | 0.0272 (12) |
| C3B $0.1074 (11)$ $0.3530 (4)$ $0.8749 (4)$ $0.0249 (11)$ H3B -0.0335 0.3907 0.8673 $0.030*$ C4B $0.1657 (9)$ $0.2974 (3)$ $0.7956 (4)$ $0.0206 (10)$ C5B $0.3589 (10)$ $0.2384 (4)$ $0.8030 (4)$ $0.0220 (11)$ H5B 0.3902 0.2010 0.7501 $0.026*$ C6B $0.5112 (10)$ $0.2353 (3)$ $0.8931 (4)$ $0.0199 (10)$ C7B $0.7150 (10)$ $0.1873 (3)$ $0.9304 (4)$ $0.0196 (10)$ C8B $0.8618 (10)$ $0.1135 (4)$ $0.8959 (4)$ $0.0216 (10)$ C9B $0.8005 (11)$ $0.0769 (4)$ $0.8031 (4)$ $0.0258 (12)$ H9B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389 (10)$ $0.0082 (4)$ $0.7720 (4)$ $0.0255 (10)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383 (12)$ $-0.0274 (4)$ $0.8297 (4)$ $0.0285 (12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968 (11)$ $0.0099 (5)$ $0.9218 (4)$ $0.0301 (11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630 (11)$ $0.0790 (4)$ $0.9549 (4)$ $0.0253 (11)$ | H2B | 0.2166 | 0.3890 | 1.0136 | 0.033* |
| H3B -0.0335 0.3907 0.8673 0.030^* C4B 0.1657 (9) 0.2974 (3) 0.7956 (4) 0.0206 (10)C5B 0.3589 (10) 0.2384 (4) 0.8030 (4) 0.0220 (11)H5B 0.3902 0.2010 0.7501 0.026^* C6B 0.5112 (10) 0.2353 (3) 0.8931 (4) 0.0199 (10)C7B 0.7150 (10) 0.1873 (3) 0.9304 (4) 0.0196 (10)C8B 0.8618 (10) 0.1135 (4) 0.8959 (4) 0.0216 (10)C9B 0.8005 (11) 0.0769 (4) 0.8031 (4) 0.0258 (12)H9B 0.6644 0.0996 0.7621 0.031^* C10B 0.9389 (10) 0.0082 (4) 0.7720 (4) 0.0255 (10)H10B 0.8969 -0.0158 0.7089 0.031^* C11B 1.1383 (12) -0.0274 (4) 0.8297 (4) 0.0285 (12)H11B 1.2315 -0.0753 0.8076 0.034^* C12B 1.1968 (11) 0.0099 (5) 0.9218 (4) 0.0301 (11)H12B 1.3328 -0.0131 0.9626 0.036^* C13B 1.0630 (11) 0.0790 (4) 0.9549 (4) 0.0253 (11)H13B 1.1071 0.1032 1.0177 0.300^* | C3B | 0.1074 (11) | 0.3530 (4) | 0.8749 (4) | 0.0249 (11) |
| C4B $0.1657 (9)$ $0.2974 (3)$ $0.7956 (4)$ $0.0206 (10)$ C5B $0.3589 (10)$ $0.2384 (4)$ $0.8030 (4)$ $0.0220 (11)$ H5B 0.3902 0.2010 0.7501 $0.026*$ C6B $0.5112 (10)$ $0.2353 (3)$ $0.8931 (4)$ $0.0199 (10)$ C7B $0.7150 (10)$ $0.1873 (3)$ $0.9304 (4)$ $0.0196 (10)$ C8B $0.8618 (10)$ $0.1135 (4)$ $0.8959 (4)$ $0.0216 (10)$ C9B $0.8005 (11)$ $0.0769 (4)$ $0.8031 (4)$ $0.0258 (12)$ H9B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389 (10)$ $0.0082 (4)$ $0.7720 (4)$ $0.0255 (10)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383 (12)$ $-0.0274 (4)$ $0.8297 (4)$ $0.0285 (12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968 (11)$ $0.0099 (5)$ $0.9218 (4)$ $0.0301 (11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630 (11)$ $0.0790 (4)$ $0.9549 (4)$ $0.0253 (11)$ H13B 1.1071 0.1032 1.0177 $0.030*$ | H3B | -0.0335 | 0.3907 | 0.8673 | 0.030* |
| C5B0.3589 (10)0.2384 (4)0.8030 (4)0.0220 (11)H5B0.39020.20100.75010.026*C6B0.5112 (10)0.2353 (3)0.8931 (4)0.0199 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C8B0.8618 (10)0.1135 (4)0.8959 (4)0.0216 (10)C9B0.8005 (11)0.0769 (4)0.8031 (4)0.0258 (12)H9B0.66440.09960.76210.031*C10B0.9389 (10)0.0082 (4)0.7720 (4)0.0255 (10)H10B0.8969-0.01580.70890.031*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | C4B | 0.1657 (9) | 0.2974 (3) | 0.7956 (4) | 0.0206 (10) |
| H5B0.39020.20100.75010.026*C6B0.5112 (10)0.2353 (3)0.8931 (4)0.0199 (10)C7B0.7150 (10)0.1873 (3)0.9304 (4)0.0196 (10)C8B0.8618 (10)0.1135 (4)0.8959 (4)0.0216 (10)C9B0.8005 (11)0.0769 (4)0.8031 (4)0.0258 (12)H9B0.66440.09960.76210.031*C10B0.9389 (10)0.0082 (4)0.7720 (4)0.0255 (10)H10B0.8969-0.01580.70890.031*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | C5B | 0.3589 (10) | 0.2384 (4) | 0.8030 (4) | 0.0220 (11) |
| C6B $0.5112 (10)$ $0.2353 (3)$ $0.8931 (4)$ $0.0199 (10)$ C7B $0.7150 (10)$ $0.1873 (3)$ $0.9304 (4)$ $0.0196 (10)$ C8B $0.8618 (10)$ $0.1135 (4)$ $0.8959 (4)$ $0.0216 (10)$ C9B $0.8005 (11)$ $0.0769 (4)$ $0.8031 (4)$ $0.0258 (12)$ H9B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389 (10)$ $0.0082 (4)$ $0.7720 (4)$ $0.0255 (10)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383 (12)$ $-0.0274 (4)$ $0.8297 (4)$ $0.0285 (12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968 (11)$ $0.0099 (5)$ $0.9218 (4)$ $0.0301 (11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630 (11)$ $0.0790 (4)$ $0.9549 (4)$ $0.0253 (11)$ H13B 1.1071 0.1032 1.0177 $0.030*$ | H5B | 0.3902 | 0.2010 | 0.7501 | 0.026* |
| C7B $0.7150(10)$ $0.1873(3)$ $0.9304(4)$ $0.0196(10)$ C8B $0.8618(10)$ $0.1135(4)$ $0.8959(4)$ $0.0216(10)$ C9B $0.8005(11)$ $0.0769(4)$ $0.8031(4)$ $0.0258(12)$ H9B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389(10)$ $0.0082(4)$ $0.7720(4)$ $0.0255(10)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383(12)$ $-0.0274(4)$ $0.8297(4)$ $0.0285(12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968(11)$ $0.0099(5)$ $0.9218(4)$ $0.0301(11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630(11)$ $0.0790(4)$ $0.9549(4)$ $0.0253(11)$ H13B 1.1071 0.1032 1.0177 $0.030*$ | C6B | 0.5112 (10) | 0.2353 (3) | 0.8931 (4) | 0.0199 (10) |
| C8B $0.8618(10)$ $0.1135(4)$ $0.8959(4)$ $0.0216(10)$ C9B $0.8005(11)$ $0.0769(4)$ $0.8031(4)$ $0.0258(12)$ H9B 0.6644 0.0996 0.7621 $0.031*$ C10B $0.9389(10)$ $0.0082(4)$ $0.7720(4)$ $0.0255(10)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383(12)$ $-0.0274(4)$ $0.8297(4)$ $0.0285(12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968(11)$ $0.0099(5)$ $0.9218(4)$ $0.0301(11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630(11)$ $0.0790(4)$ $0.9549(4)$ $0.0253(11)$ H13B 1.1071 0.1032 1.0177 $0.030*$ | C7B | 0.7150 (10) | 0.1873 (3) | 0.9304 (4) | 0.0196 (10) |
| C9B $0.8005 (11)$ $0.0769 (4)$ $0.8031 (4)$ $0.0258 (12)$ H9B 0.6644 0.0996 0.7621 0.031^* C10B $0.9389 (10)$ $0.0082 (4)$ $0.7720 (4)$ $0.0255 (10)$ H10B 0.8969 -0.0158 0.7089 0.031^* C11B $1.1383 (12)$ $-0.0274 (4)$ $0.8297 (4)$ $0.0285 (12)$ H11B 1.2315 -0.0753 0.8076 0.034^* C12B $1.1968 (11)$ $0.0099 (5)$ $0.9218 (4)$ $0.0301 (11)$ H12B 1.3328 -0.0131 0.9626 0.036^* C13B $1.0630 (11)$ $0.0790 (4)$ $0.9549 (4)$ $0.0253 (11)$ H13B 1.1071 0.1032 1.0177 0.030^* | C8B | 0.8618 (10) | 0.1135 (4) | 0.8959 (4) | 0.0216 (10) |
| H9B0.66440.09960.76210.031*C10B0.9389 (10)0.0082 (4)0.7720 (4)0.0255 (10)H10B0.8969-0.01580.70890.031*C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | C9B | 0.8005 (11) | 0.0769 (4) | 0.8031 (4) | 0.0258 (12) |
| C10B $0.9389(10)$ $0.0082(4)$ $0.7720(4)$ $0.0255(10)$ H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B $1.1383(12)$ $-0.0274(4)$ $0.8297(4)$ $0.0285(12)$ H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B $1.1968(11)$ $0.0099(5)$ $0.9218(4)$ $0.0301(11)$ H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B $1.0630(11)$ $0.0790(4)$ $0.9549(4)$ $0.0253(11)$ H13B 1.1071 0.1032 1.0177 $0.030*$ | H9B | 0.6644 | 0.0996 | 0.7621 | 0.031* |
| H10B 0.8969 -0.0158 0.7089 $0.031*$ C11B 1.1383 (12) -0.0274 (4) 0.8297 (4) 0.0285 (12)H11B 1.2315 -0.0753 0.8076 $0.034*$ C12B 1.1968 (11) 0.0099 (5) 0.9218 (4) 0.0301 (11)H12B 1.3328 -0.0131 0.9626 $0.036*$ C13B 1.0630 (11) 0.0790 (4) 0.9549 (4) 0.0253 (11)H13B 1.1071 0.1032 1.0177 $0.030*$ | C10B | 0.9389 (10) | 0.0082 (4) | 0.7720 (4) | 0.0255 (10) |
| C11B1.1383 (12)-0.0274 (4)0.8297 (4)0.0285 (12)H11B1.2315-0.07530.80760.034*C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | H10B | 0.8969 | -0.0158 | 0.7089 | 0.031* |
| H11B1.2315-0.07530.80760.034*C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | C11B | 1.1383 (12) | -0.0274 (4) | 0.8297 (4) | 0.0285 (12) |
| C12B1.1968 (11)0.0099 (5)0.9218 (4)0.0301 (11)H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | H11B | 1.2315 | -0.0753 | 0.8076 | 0.034* |
| H12B1.3328-0.01310.96260.036*C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | C12B | 1.1968 (11) | 0.0099 (5) | 0.9218 (4) | 0.0301 (11) |
| C13B1.0630 (11)0.0790 (4)0.9549 (4)0.0253 (11)H13B1.10710.10321.01770.030* | H12B | 1.3328 | -0.0131 | 0.9626 | 0.036* |
| H13B 1.1071 0.1032 1.0177 0.030* | C13B | 1.0630 (11) | 0.0790 (4) | 0.9549 (4) | 0.0253 (11) |
| | H13B | 1.1071 | 0.1032 | 1.0177 | 0.030* |

| O1A | 0.028 (2) | 0.021 (2) | 0.031 (2) | 0.0056 (16) | 0.0085 (17) | 0.0011 (16) |
|------|--------------|--------------|--------------|--------------|---------------|--------------|
| N1A | 0.036 (3) | 0.024 (2) | 0.037 (3) | -0.001 (3) | 0.014 (2) | 0.007 (2) |
| C1A | 0.010 (2) | 0.055 (4) | 0.011 (2) | 0.000 (2) | -0.0008 (18) | 0.000 (2) |
| C2A | 0.029 (3) | 0.033 (3) | 0.030 (3) | -0.001 (3) | 0.006 (2) | 0.011 (2) |
| C3A | 0.029 (3) | 0.028 (3) | 0.022 (3) | 0.001 (2) | 0.006 (2) | 0.004 (2) |
| C4A | 0.021 (3) | 0.025 (3) | 0.020 (2) | 0.006 (2) | -0.0003 (19) | -0.002(2) |
| C5A | 0.021 (3) | 0.015 (2) | 0.025 (3) | 0.000(2) | 0.001 (2) | -0.0027 (19) |
| C6A | 0.021 (3) | 0.018 (3) | 0.021 (3) | 0.000 (2) | 0.001 (2) | 0.0002 (19) |
| C7A | 0.020 (3) | 0.021 (3) | 0.022 (3) | 0.001 (2) | -0.003 (2) | 0.0008 (19) |
| C8A | 0.021 (2) | 0.023 (3) | 0.017 (2) | 0.001 (2) | 0.0032 (19) | -0.0026 (19) |
| C9A | 0.042 (3) | 0.018 (3) | 0.019 (2) | 0.005 (3) | 0.005 (2) | -0.001 (2) |
| C10A | 0.039 (3) | 0.017 (3) | 0.024 (3) | -0.001 (2) | 0.000 (2) | 0.002 (2) |
| C11A | 0.021 (3) | 0.048 (4) | 0.020 (3) | -0.012 (2) | 0.001 (2) | 0.008 (2) |
| C12A | 0.020 (3) | 0.026 (3) | 0.023 (3) | 0.000 (2) | 0.000 (2) | -0.003 (2) |
| C13A | 0.020 (3) | 0.025 (3) | 0.021 (3) | 0.003 (2) | 0.001 (2) | -0.002(2) |
| I1B | 0.02550 (18) | 0.02499 (18) | 0.03013 (19) | 0.00099 (17) | -0.00173 (14) | 0.00057 (16) |
| O1B | 0.032 (2) | 0.028 (2) | 0.0171 (19) | -0.0014 (18) | 0.0017 (15) | -0.0014 (16) |
| N1B | 0.035 (3) | 0.021 (2) | 0.025 (2) | -0.0026 (19) | 0.004 (2) | 0.0006 (17) |
| C1B | 0.030 (3) | 0.022 (3) | 0.019 (2) | -0.005 (2) | 0.007 (2) | 0.0006 (18) |
| C2B | 0.027 (3) | 0.026 (3) | 0.030 (3) | -0.003 (2) | 0.012 (2) | 0.001 (2) |
| C3B | 0.021 (3) | 0.024 (3) | 0.032 (3) | 0.000 (2) | 0.009 (2) | -0.001 (2) |
| C4B | 0.022 (2) | 0.018 (3) | 0.022 (2) | -0.004 (2) | 0.0011 (19) | 0.0015 (18) |
| C5B | 0.023 (3) | 0.021 (3) | 0.022 (3) | -0.004 (2) | 0.003 (2) | -0.0012 (19) |
| C6B | 0.021 (3) | 0.018 (2) | 0.021 (3) | -0.003 (2) | 0.005 (2) | -0.0020 (18) |
| C7B | 0.023 (3) | 0.017 (2) | 0.019 (2) | -0.005 (2) | 0.002 (2) | 0.0018 (18) |
| C8B | 0.020 (3) | 0.019 (2) | 0.026 (3) | -0.003 (2) | 0.003 (2) | 0.003 (2) |
| C9B | 0.024 (3) | 0.028 (3) | 0.025 (3) | 0.000 (2) | 0.000 (2) | 0.001 (2) |
| C10B | 0.026 (3) | 0.025 (3) | 0.026 (2) | 0.002 (3) | 0.0045 (19) | -0.004 (2) |
| C11B | 0.029 (3) | 0.026 (3) | 0.031 (3) | 0.003 (2) | 0.009 (2) | 0.004 (2) |
| C12B | 0.029 (3) | 0.031 (3) | 0.029 (3) | 0.005 (3) | -0.003 (2) | 0.006 (3) |
| C13B | 0.027 (3) | 0.028 (3) | 0.020 (3) | 0.001 (2) | -0.002 (2) | 0.002 (2) |

Geometric parameters (Å, °)

| IIA—C4A | 2.100 (5) | I1B—C4B | 2.100 (5) |
|---------|-----------|----------|-----------|
| O1A—C7A | 1.354 (6) | O1B—C7B | 1.366 (6) |
| O1A—N1A | 1.413 (6) | O1B—N1B | 1.397 (6) |
| N1A—C1A | 1.346 (8) | N1B—C1B | 1.329 (8) |
| C1A—C6A | 1.361 (8) | C1B—C6B | 1.427 (7) |
| C1A—C2A | 1.462 (8) | C1B—C2B | 1.430 (8) |
| C2A—C3A | 1.344 (9) | C2B—C3B | 1.363 (9) |
| C2A—H2A | 0.9500 | C2B—H2B | 0.9500 |
| C3A—C4A | 1.430 (8) | C3B—C4B | 1.437 (8) |
| СЗА—НЗА | 0.9500 | C3B—H3B | 0.9500 |
| C4A—C5A | 1.362 (7) | C4B—C5B | 1.371 (8) |
| C5A—C6A | 1.432 (7) | C5B—C6B | 1.426 (8) |
| C5A—H5A | 0.9500 | C5B—H5B | 0.9500 |
| C6A—C7A | 1.387 (7) | C6B—C7B | 1.379 (7) |
| C7A—C8A | 1.466 (7) | C7B—C8B | 1.475 (8) |
| C8A—C9A | 1.405 (8) | C8B—C13B | 1.398 (8) |
| | | | |

| C8A—C13A | 1.405 (7) | C8B—C9B | 1.406 (8) |
|-------------------------------------|----------------------|-------------------------------------|----------------------|
| C9A—C10A | 1.387 (8) | C9B—C10B | 1.374 (8) |
| C9A—H9A | 0.9500 | C9B—H9B | 0.9500 |
| C10A - C11A | 1 362 (8) | C10B-C11B | 1 389 (8) |
| C10A - H10A | 0.9500 | C10B - H10B | 0.9500 |
| $C_{11}A - C_{12}A$ | 1 420 (9) | C11B - C12B | 1 399 (9) |
| $C_{11}A - H_{11}A$ | 0.9500 | C11B—H11B | 0.9500 |
| C12A - C13A | 1 384 (8) | C12B $C13B$ | 1 374 (9) |
| C12A = C13A | 0.9500 | C12B H12B | 0.0500 |
| C12A—III2A C13A H13A | 0.9500 | C12B H13B | 0.9500 |
| CI3A—III3A | 0.9500 | | 0.9500 |
| C7A—01A—N1A | 110.0 (4) | C7B—O1B—N1B | 110.9 (4) |
| C1A—N1A—O1A | 102.4 (5) | C1B—N1B—O1B | 104.3 (4) |
| N1A—C1A—C6A | 114.9 (5) | N1B—C1B—C6B | 112.5 (5) |
| N1A—C1A—C2A | 121.2 (6) | N1B—C1B—C2B | 126.5 (5) |
| C6A—C1A—C2A | 123.9 (6) | C6B—C1B—C2B | 121.0 (5) |
| C3A—C2A—C1A | 115.1 (6) | C3B—C2B—C1B | 118.3 (5) |
| C3A—C2A—H2A | 122.5 | C3B—C2B—H2B | 120.8 |
| C1A—C2A—H2A | 122.5 | C1B—C2B—H2B | 120.8 |
| C2A - C3A - C4A | 121 7 (5) | C^2B — C^3B — C^4B | 120.4(5) |
| C2A - C3A - H3A | 119.1 | C2B $C3B$ $C1BC2B$ $C3B$ $H3B$ | 119.8 |
| C4A - C3A - H3A | 119.1 | C4B-C3B-H3B | 119.8 |
| C_{5A} C_{4A} C_{3A} | 122.9 (5) | C5B-C4B-C3B | 122.9(5) |
| C_{5A} C_{4A} U_{1A} | 122.9(3) 1197(4) | C5B - C4B - U1B | 122.9(3) 118.4(4) |
| C_{3A} C_{4A} I_{1A} | 117.7(4) 117.4(4) | C_{3B} C_{4B} I_{1B} | 110.4(+) 118.7(4) |
| C_{AA} C_{AA} C_{AA} C_{AA} | 117.4 (4) | $C_{3}D_{-}C_{4}D_{-}HD_{-}$ | 110.7(+) 117.5(5) |
| $C_{4A} = C_{5A} = C_{6A}$ | 121 4 | C4B $C5B$ $H5B$ | 121.2 |
| $C_{4A} = C_{5A} = H_{5A}$ | 121.4 | C4D = C5D = H5D | 121.2 |
| $C_{0A} = C_{0A} = M_{0A}$ | 121.4 | C7P $C6P$ $C5P$ | 121.2 136.0 (5) |
| C1A = C6A = C5A | 104.0(5) | C7B = C6B = C1B | 104.2(5) |
| CTA = CGA = CSA | 119.2(3) 126.8(5) | $C_{D} = C_{D} = C_{D}$ | 104.2(3) |
| C/A = COA = CSA | 130.0(3) 108.7(5) | C_{3B} C_{0B} C_{1B} C_{6B} | 119.0(3) 109.0(4) |
| O1A C7A C8A | 106.7(3) | O1B - C7B - C0B | 106.0(4) |
| OIA - C/A - CoA | 110.4(3) | $OIB - C/B - C\delta B$ | 110.5(3) |
| COA = C/A = COA | 134.9 (5) | C_{0B} C_{B} C_{0B} C_{0B} | 133.0 (5) |
| C9A = C8A = C7A | 119.0 (5) | C13B = C8B = C9B | 119.2 (5) |
| C9A - C8A - C7A | 120.9 (5) | | 120.6 (5) |
| C13A - C8A - C/A | 120.1 (5) | C9B—C8B—C7B | 120.2 (5) |
| C10A—C9A—C8A | 120.5 (5) | C10B—C9B—C8B | 119.6 (6) |
| C10A—C9A—H9A | 119.8 | C10B—C9B—H9B | 120.2 |
| С8А—С9А—Н9А | 119.8 | С8В—С9В—Н9В | 120.2 |
| C11A—C10A—C9A | 121.2 (5) | C9B—C10B—C11B | 122.1 (6) |
| C11A—C10A—H10A | 119.4 | C9B—C10B—H10B | 118.9 |
| C9A—C10A—H10A | 119.4 | C11B—C10B—H10B | 118.9 |
| C10A—C11A—C12A | 118.9 (5) | C10B—C11B—C12B | 117.5 (6) |
| C10A—C11A—H11A | 120.5 | C10B—C11B—H11B | 121.3 |
| C12A—C11A—H11A | 120.5 | C12B—C11B—H11B | 121.3 |
| C13A—C12A—C11A | 120.9 (5) | C13B—C12B—C11B | 121.8 (5) |
| C13A—C12A—H12A | 119.6 | C13B—C12B—H12B | 119.1 |
| C11A—C12A—H12A | 119.6 | C11B—C12B—H12B | 119.1 |

| C12A—C13A—C8A | 119.5 (5) | C12B—C13B—C8B | 119.8 (5) |
|----------------|-----------|----------------|-----------|
| C12A—C13A—H13A | 120.3 | C12B—C13B—H13B | 120.1 |
| C8A—C13A—H13A | 120.3 | C8B—C13B—H13B | 120.1 |

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C1B–C6B ring.

| D—H···A | <i>D</i> —Н | H···A | $D \cdots A$ | <i>D</i> —H…A |
|---|-------------|----------|--------------|---------------|
| $C3A$ — $H3A$ ···N1 B^{i} | 0.95 | 2.40 | 3.247 (7) | 149 |
| $C11A$ — $H11A$ ···N $1A^{ii}$ | 0.95 | 2.47 | 3.339 (8) | 152 |
| C4A—I1A···Cg ⁱⁱⁱ | 2.10(1) | 3.62 (1) | 5.637 (6) | 160 (1) |
| C4 <i>B</i> —I1 <i>B</i> ···O1 <i>A</i> | 2.10(1) | 3.34 (1) | 5.325 (7) | 156 (1) |

Symmetry codes: (i) *x*, *y*, *z*-1; (ii) -*x*-1, *y*-1/2, -*z*+1; (iii) -*x*+1, *y*-1/2, -*z*+1.