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(2-Aminoethoxy)bis(2-thienyl)boron

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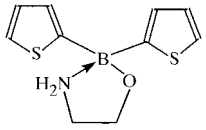
In the five-membered ring in the title compound, (2-aminoethoxy)bis(2-thienyl)boron, $C_{10}H_{12}BNOS_2$, the B atom is four-coordinate with dimensions N—B 1.654 (3), O—B 1.479 (3), and C—B 1.606 (3) and 1.609 (3) Å. An intermolecular hydrogen bond between an amino H atom and the ethoxy O atom links the molecules into infinite chains along the *a* axis. Only one of the two amino H atoms is involved in hydrogen bonding because there is only the one acceptor atom, the ethoxy O atom, and the molecular geometry precludes formation of a second hydrogen bond by the second amino H atom.

Comment

Examination of the title structure, (I), with *PLATON* (Spek, 1999) showed that there were no solvent-accessible voids in the crystal lattice.



(I)

Experimental

The title compound was prepared according to a published procedure (Coutts & Musgrave, 1970) from 2-aminoethanol and bis(2-thienyl)boronic acid, which was obtained from $(BuO)_3B$ and 2-BrMg-thiophene (m.p. 474–476 K; literature value 473–475 K).

Crystal data

$C_{10}H_{12}BNOS_2$
M_r = 237.14
Orthorhombic, *Pbca*
a = 10.0818 (3) Å
b = 16.1220 (7) Å
c = 13.7747 (6) Å
V = 2238.92 (15) Å^3
Z = 8
D_x = 1.407 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2562 reflections
θ = 2.52–27.43°
μ = 0.445 mm^{-1}
T = 150.0 (1) K
Plate, colourless
0.20 × 0.15 × 0.05 mm

Data collection

KappaCCD diffractometer
φ and ω scans with κ offset scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.916, T_{max} = 0.978
15 841 measured reflections
2562 independent reflections
1888 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 27.43°
h = −12 → 12
k = −20 → 20
l = −17 → 17

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 1.063
2562 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.4651P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Molecule (I) crystallized in the orthorhombic system; space group Pbca from the systematic absences. H atoms were treated as riding atoms with C—H 0.95–0.99 Å and N—H 0.92 Å.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC, X-ray Crystallographic Service, University of Southampton, using an Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all there help and advice.

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