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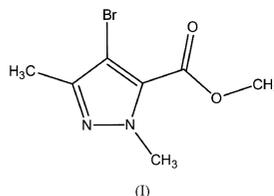
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**Key indicators**Single-crystal X-ray study  
 $T = 183\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.035  
 $wR$  factor = 0.079  
Data-to-parameter ratio = 14.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**Methyl 4-bromo-1,3-dimethylpyrazole-5-carboxylate**

The crystal structure of the title compound,  $\text{C}_7\text{H}_9\text{BrN}_2\text{O}_2$ , has been determined in the triclinic space group  $P\bar{1}$ . There are three molecules in the asymmetric unit, arranged with approximate threefold rotation symmetry, and the three pyrazole rings are almost coplanar. A bromine atom at the 4-position of the pyrazole ring provides the possibility for synthesis of substituted pyrazole derivatives. Packing is governed only by van der Waals interactions.

**Comment**

As a functional compound, the title compound, (I), is useful in organic synthesis. The ester group at C3 can be reduced to a hydroxymethyl group by  $\text{LiAlH}_4$  (Schenck *et al.*, 1985). The existence of a bromine atom at C2 affords the possibility for the molecule to form new C–C bonds through the Suzuki cross-coupling reaction (Yin *et al.*, 2002), with a series of aromatic boron compounds, making it a useful intermediate for organic synthesis.



The molecular structure and crystal packing are illustrated in Figs 1 and 2. Selected geometric parameters are listed in Table 1. Inspection of these values indicates that there is delocalization of the  $\pi$ -electron density in the pyrazole ring. There are three molecules in the asymmetric unit and the three pyrazole rings are nearly coplanar; they are related by an approximate threefold rotation axis. The independent molecules have different dihedral angles between the pyrazole ring planes and the ester planes,  $\text{O}=\text{C}-\text{O}$ . The dihedral angles formed by the pyrazole rings and the attached ester groups are  $3.9$  (6),  $10.2$  (5) and  $6.4$  (7) $^\circ$  for the C1, C1A and C1B molecules, respectively. The displacements of atoms Br1, C5, C7 from the pyrazole planes are in the range  $0.005$  (4)– $0.095$  (5)  $\text{\AA}$ . These displacements are probably caused by neighbouring interactions. All bond lengths are normal, but there are distortions in the exocyclic bond angles (Table 1). These may be caused by steric interactions involving the bromine atoms in particular. The packing is governed only by van der Waals interactions.

**Experimental**

The title compound was prepared by alkylation of 4-bromo-3-methylpyrazole-5-carboxylic acid (Chambers & Denny, 1985), which

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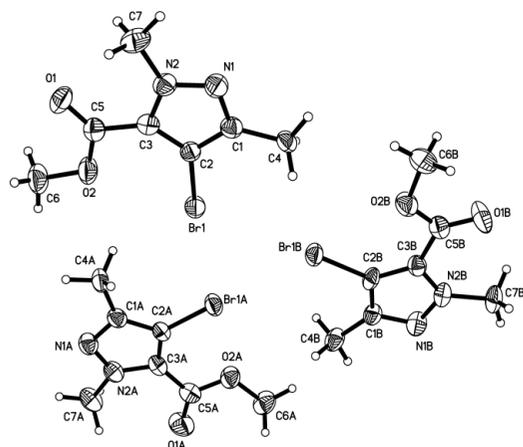


Figure 1

A view of the three molecules in the asymmetric unit. Ellipsoids are drawn at the 50% probability level.

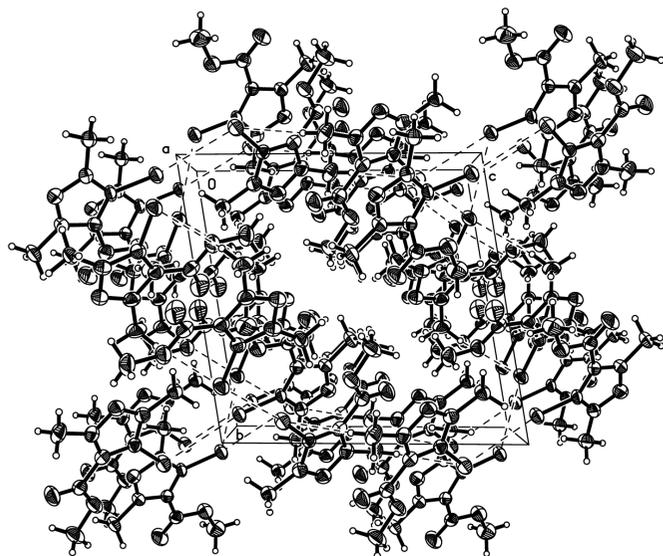


Figure 2

The packing of (I), viewed down the *a* axis.

was synthesized by bromination of 3-methylpyrazole-5-carboxylic acid in aqueous solution. To 4-bromo-3-methylpyrazole-5-carboxylic acid in anhydrous acetone solution was added dimethyl sulfate and anhydrous potassium carbonate, and the mixture was stirred at the boiling point for 24 h. The mixture was filtered and the filtrate evaporated to dryness. Crystallization from Et<sub>2</sub>O/petroleum gave the title compound. The yield of the product was 76% (m.p. 330 K). Crystals suitable for single-crystal X-ray diffraction analysis were grown from a CCl<sub>4</sub> (3 ml) solution of the compound (100 mg) at room temperature.

#### Crystal data

C<sub>7</sub>H<sub>9</sub>BrN<sub>2</sub>O<sub>2</sub>  
*M<sub>r</sub>* = 233.07  
 Triclinic, *P* $\bar{1}$   
*a* = 10.226 (2) Å  
*b* = 11.207 (2) Å  
*c* = 11.778 (2) Å  
 $\alpha$  = 80.75 (3)°  
 $\beta$  = 85.32 (3)°  
 $\gamma$  = 88.70 (3)°  
*V* = 1327.7 (5) Å<sup>3</sup>

*Z* = 6  
*D<sub>x</sub>* = 1.749 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation  
 Cell parameters from 7285 reflections  
 $\theta$  = 2.3–26.1°  
 $\mu$  = 4.61 mm<sup>-1</sup>  
*T* = 183 (2) K  
 Block, colorless  
 0.40 × 0.20 × 0.20 mm

#### Data collection

Bruker SMART 1K CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T*<sub>min</sub> = 0.226, *T*<sub>max</sub> = 0.398  
 5487 measured reflections

4564 independent reflections  
 3338 reflections with *I* > 2 $\sigma$ (*I*)  
*R*<sub>int</sub> = 0.018  
 $\theta$ <sub>max</sub> = 25.0°  
*h* = −12 → 6  
*k* = −13 → 11  
*l* = −14 → 13

#### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.035  
*wR*(*F*<sup>2</sup>) = 0.079  
*S* = 0.97  
 4564 reflections  
 325 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.033P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.45 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.47 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

N1—C1	1.331 (5)	N2A—C3A	1.357 (5)
C1—C2	1.389 (5)	N1A—N2A	1.342 (5)
C2—C3	1.378 (5)	N1B—C1B	1.345 (5)
N2—C3	1.356 (5)	C1B—C2B	1.392 (6)
N1—N2	1.344 (4)	C2B—C3B	1.371 (5)
N1A—C1A	1.343 (5)	N2B—C3B	1.357 (5)
C1A—C2A	1.405 (5)	N1B—N2B	1.335 (5)
C2A—C3A	1.371 (6)		
C2—C1—C4	129.0 (4)	C2A—C3A—C5A	132.9 (4)
N1—C1—C4	121.1 (4)	N2A—C3A—C5A	121.4 (4)
C3—C2—Br1	129.0 (3)	C3A—N2A—C7A	130.4 (4)
C1—C2—Br1	124.3 (3)	N1A—N2A—C7A	117.3 (3)
C2—C3—C5	133.8 (4)	C2B—C1B—C4B	130.1 (3)
N2—C3—C5	120.8 (4)	N1B—C1B—C4B	120.6 (4)
C3—N2—C7	130.1 (4)	C3B—C2B—Br1B	129.3 (3)
N1—N2—C7	117.8 (3)	C1B—C2B—Br1B	123.2 (3)
C2A—C1A—C4A	129.8 (4)	C2B—C3B—C5B	133.2 (4)
N1A—C1A—C4A	121.7 (4)	N2B—C3B—C5B	122.3 (4)
C3A—C2A—Br1A	129.8 (3)	C3B—N2B—C7B	128.8 (4)
C1A—C2A—Br1A	122.8 (3)	N1B—N2B—C7B	117.7 (4)

H atoms were placed in geometrically idealized positions, with C—H = 0.98 Å, and were constrained to ride on their parent atoms, with *U*<sub>iso</sub> = 1.5*U*<sub>eq</sub>(C).

Data collection: SMART (Bruker, 2000); cell refinement: SMART; data reduction: SAINT and SHELXTL (Bruker, 2000); program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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