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## Structure Reports

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**(E)-1-Bromo-4-(2-nitroprop-1-enyl)-benzene**

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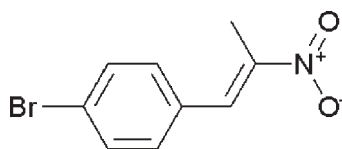
Received 11 November 2009; accepted 17 November 2009

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.035;  $wR$  factor = 0.094; data-to-parameter ratio = 17.6.

The title compound,  $\text{C}_9\text{H}_8\text{BrNO}_2$ , which was synthesized by the condensation of 4-bromobenzaldehyde with nitroethane, possesses a *trans* configuration. The dihedral angle between the benzene ring and the mean plane of the double bond is  $7.31$  (3)°. The crystal structure is stabilized by short intermolecular  $\text{Br} \cdots \text{O}$  contacts [3.168 (4) Å].

## Related literature

For general background to nitroalkenes as intermediates in the preparation of numerous products including insecticides and pharmacologically active substances, see: Boelle *et al.* (1998); Vallejos *et al.* (2005). For related structures, see: Boys *et al.* (1993); Mugnoli *et al.* (1991).



## Experimental

## Crystal data

 $\text{C}_9\text{H}_8\text{BrNO}_2$  $M_r = 242.07$ 

Triclinic,  $P\bar{1}$   
 $a = 6.9787$  (5) Å  
 $b = 7.4123$  (5) Å  
 $c = 9.7659$  (6) Å  
 $\alpha = 105.435$  (2)°  
 $\beta = 95.087$  (2)°  
 $\gamma = 104.323$  (2)°

$V = 465.31$  (5) Å<sup>3</sup>  
 $Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 4.38$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.21 \times 0.19 \times 0.08$  mm

## Data collection

Rigaku R-Axis RAPID  
diffractometer  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.388$ ,  $T_{\max} = 0.703$

4605 measured reflections  
2112 independent reflections  
1303 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.094$   
 $S = 1.00$   
2112 reflections

120 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.46$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.71$  e Å<sup>-3</sup>

Data collection: *PROCESS-AUTO* (Rigaku, 2006); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2017).

## References

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## supporting information

*Acta Cryst.* (2009). E65, o3174 [doi:10.1107/S1600536809048910]

**(E)-1-Bromo-4-(2-nitroprop-1-enyl)benzene****Bailin Li****S1. Comment**

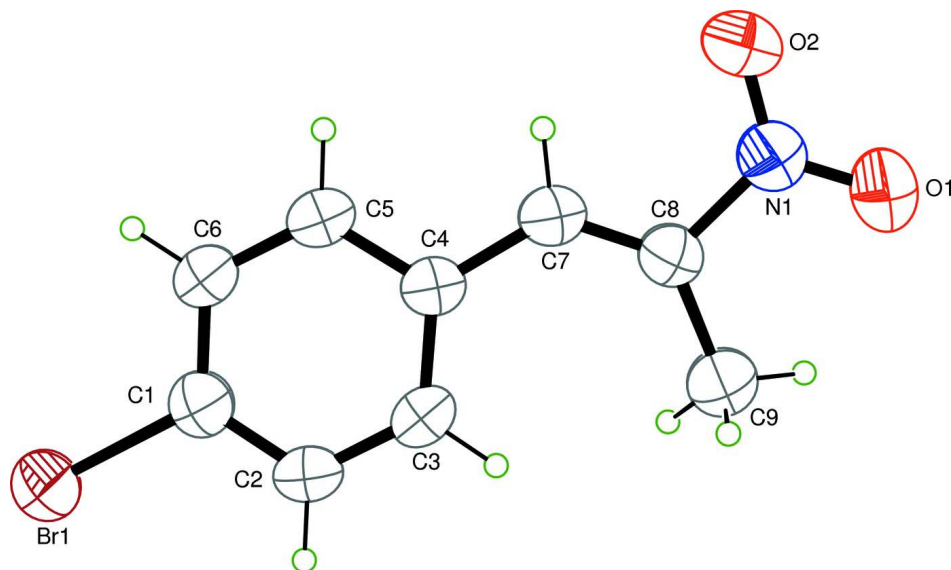
Nitroalkenes are valuable intermediates for preparation of numerous products including insecticides and pharmacologically active substances (Boelle *et al.*, 1998 and Vallejos *et al.*, 2005) in which the nitro group can be easily transformed into a variety of groups with different functionalities, such as amine, carbonyl groups, *etc.*. In this article, the crystal structure of the title compound (*E*)-1-bromo-4-(2-nitroprop-1-enyl)benzene is presented (Fig. 1). The dihedral angle between the benzene ring and the mean plan of the double bond H7/C7/C8/C9 is 7.31 (3) °. The crystal structure is stabilized by short intermolecular Br—O contacts [3.168 (4) Å].

**S2. Experimental**

To a solution of 4-bromobenzaldehyde (50 mmol) in AcOH (25 ml), nitroethane (75 mmol) was added, followed by butylamine (100 mmol, 7.4 ml). The mixture was sonicated at 333 K, until TLC showed full conversion of aldehyde. The mixture was poured into ice water, the precipitate was filtered off, washed with water and recrystallized from EtOH to give (*E*)-1-bromo-4-(2-nitroprop-1-enyl)benzene. Suitable crystals of the title compound were obtained by slow evaporation of an ethanol solution at room temperature.

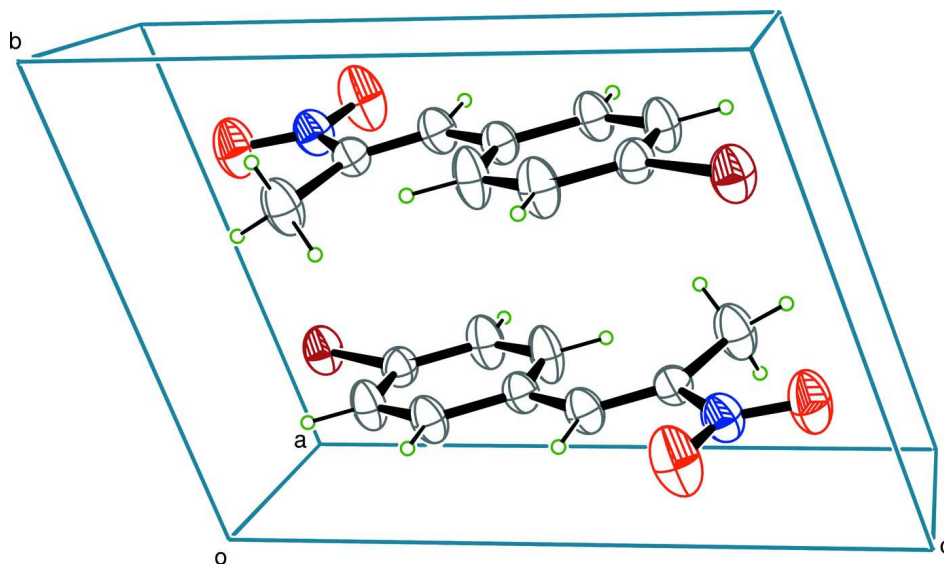
**S3. Refinement**

All carbon-bonded H atoms were placed in calculated positions with C—H = 0.93 Å (aromatic), C—H = 0.96 Å (*sp*) and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2_{\text{eq}}(\text{C})$ .



**Figure 1**

The asymmetric unit of the title compound (I) with the atomic labeling scheme. Displacement ellipsoids are drawn at the 40% probability level.



**Figure 2**

Molecular packing of the title compound (I) viewed down the *a* axis.

**(*E*)-1-Bromo-4-(2-nitroprop-1-enyl)benzene**

*Crystal data*

$C_9H_8BrNO_2$

$M_r = 242.07$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 6.9787$  (5) Å

$b = 7.4123$  (5) Å

$c = 9.7659$  (6) Å

$\alpha = 105.435$  (2)°

$\beta = 95.087$  (2)°

$\gamma = 104.323$  (2)°

$V = 465.31$  (5) Å<sup>3</sup>

$Z = 2$

$F(000) = 240$

$D_x = 1.728$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 3184 reflections  
 $\theta = 3.1\text{--}27.4^\circ$   
 $\mu = 4.38 \text{ mm}^{-1}$

$T = 296 \text{ K}$   
 Platelet, yellow  
 $0.21 \times 0.19 \times 0.08 \text{ mm}$

*Data collection*

Rigaku R-AXIS RAPID  
 diffractometer  
 Radiation source: rolling anode  
 Graphite monochromator  
 Detector resolution:  $10.00 \text{ pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.388$ ,  $T_{\max} = 0.703$

4605 measured reflections  
 2112 independent reflections  
 1303 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$   
 $\theta_{\max} = 27.4^\circ$ ,  $\theta_{\min} = 3.1^\circ$   
 $h = -9 \rightarrow 9$   
 $k = -9 \rightarrow 8$   
 $l = -12 \rightarrow 12$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.094$   
 $S = 1.00$   
 2112 reflections  
 120 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods  
 Secondary atom site location: difference Fourier  
 map

Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.012P)^2 + 0.950P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.46 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.71 \text{ e \AA}^{-3}$   
 Extinction correction: SHELXL97 (Sheldrick,  
 2008),  $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.0149 (13)

*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.

**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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.90197 (7)	0.24927 (9)	0.09032 (5)	0.0754 (2)
N1	0.2076 (6)	0.2311 (6)	0.7592 (4)	0.0660 (10)
O1	0.2341 (5)	0.2609 (6)	0.8891 (4)	0.0937 (12)
O2	0.0411 (5)	0.1719 (7)	0.6875 (4)	0.1038 (14)
C8	0.3870 (6)	0.2659 (6)	0.6875 (4)	0.0514 (9)
C1	0.7334 (6)	0.2408 (6)	0.2327 (4)	0.0567 (10)
C5	0.4097 (6)	0.1824 (7)	0.2989 (4)	0.0631 (12)
H5	0.2712	0.1456	0.2720	0.076*
C7	0.3513 (6)	0.2154 (7)	0.5461 (4)	0.0594 (11)
H7	0.2165	0.1633	0.5051	0.071*

C4	0.4907 (6)	0.2283 (6)	0.4430 (4)	0.0524 (10)
C3	0.6976 (6)	0.2770 (8)	0.4767 (5)	0.0776 (15)
H3	0.7569	0.3055	0.5720	0.093*
C9	0.5777 (7)	0.3501 (9)	0.7900 (5)	0.0825 (16)
H9A	0.6349	0.2476	0.7987	0.099*
H9B	0.5528	0.4165	0.8825	0.099*
H9C	0.6694	0.4409	0.7555	0.099*
C2	0.8179 (6)	0.2840 (8)	0.3723 (5)	0.0742 (14)
H2	0.9565	0.3183	0.3976	0.089*
C6	0.5299 (6)	0.1901 (7)	0.1943 (4)	0.0680 (13)
H6	0.4727	0.1609	0.0985	0.082*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.0560 (3)	0.1058 (5)	0.0598 (3)	0.0136 (2)	0.0153 (2)	0.0237 (3)
N1	0.055 (2)	0.081 (3)	0.055 (2)	0.0147 (19)	0.0103 (18)	0.014 (2)
O1	0.076 (2)	0.142 (4)	0.056 (2)	0.019 (2)	0.0205 (17)	0.025 (2)
O2	0.0467 (19)	0.173 (4)	0.074 (2)	0.017 (2)	0.0114 (17)	0.020 (2)
C8	0.045 (2)	0.056 (3)	0.050 (2)	0.0112 (18)	0.0092 (17)	0.0142 (19)
C1	0.052 (2)	0.066 (3)	0.052 (2)	0.013 (2)	0.0100 (19)	0.019 (2)
C5	0.042 (2)	0.087 (3)	0.050 (2)	0.012 (2)	-0.0015 (18)	0.012 (2)
C7	0.043 (2)	0.077 (3)	0.051 (2)	0.015 (2)	0.0032 (17)	0.012 (2)
C4	0.042 (2)	0.064 (3)	0.048 (2)	0.0140 (19)	0.0039 (16)	0.013 (2)
C3	0.050 (2)	0.134 (5)	0.044 (2)	0.024 (3)	-0.0013 (19)	0.022 (3)
C9	0.052 (3)	0.122 (5)	0.055 (3)	0.008 (3)	0.003 (2)	0.015 (3)
C2	0.038 (2)	0.123 (4)	0.055 (3)	0.018 (2)	0.0015 (19)	0.022 (3)
C6	0.047 (2)	0.103 (4)	0.045 (2)	0.013 (2)	0.0013 (18)	0.017 (2)

*Geometric parameters (Å, °)*

Br1—C1	1.902 (4)	C7—C4	1.466 (5)
N1—O2	1.214 (5)	C7—H7	0.9300
N1—O1	1.217 (4)	C4—C3	1.385 (6)
N1—C8	1.488 (5)	C3—C2	1.380 (6)
C8—C7	1.314 (5)	C3—H3	0.9300
C8—C9	1.478 (6)	C9—H9A	0.9600
C1—C2	1.357 (6)	C9—H9B	0.9600
C1—C6	1.366 (6)	C9—H9C	0.9600
C5—C6	1.381 (6)	C2—H2	0.9300
C5—C4	1.388 (5)	C6—H6	0.9300
C5—H5	0.9300		
O2—N1—O1	122.1 (4)	C5—C4—C7	117.7 (4)
O2—N1—C8	119.7 (4)	C2—C3—C4	121.6 (4)
O1—N1—C8	118.2 (4)	C2—C3—H3	119.2
C7—C8—C9	130.9 (4)	C4—C3—H3	119.2
C7—C8—N1	115.8 (4)	C8—C9—H9A	109.5

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C9—C8—N1	113.2 (3)	C8—C9—H9B	109.5
C2—C1—C6	120.5 (4)	H9A—C9—H9B	109.5
C2—C1—Br1	119.2 (3)	C8—C9—H9C	109.5
C6—C1—Br1	120.3 (3)	H9A—C9—H9C	109.5
C6—C5—C4	121.6 (4)	H9B—C9—H9C	109.5
C6—C5—H5	119.2	C1—C2—C3	119.9 (4)
C4—C5—H5	119.2	C1—C2—H2	120.0
C8—C7—C4	130.1 (4)	C3—C2—H2	120.0
C8—C7—H7	115.0	C1—C6—C5	119.5 (4)
C4—C7—H7	115.0	C1—C6—H6	120.2
C3—C4—C5	116.9 (4)	C5—C6—H6	120.2
C3—C4—C7	125.4 (4)		
O2—N1—C8—C7	-4.8 (6)	C8—C7—C4—C5	-173.5 (5)
O1—N1—C8—C7	174.2 (5)	C5—C4—C3—C2	1.5 (8)
O2—N1—C8—C9	176.1 (5)	C7—C4—C3—C2	179.4 (5)
O1—N1—C8—C9	-4.9 (6)	C6—C1—C2—C3	-0.1 (8)
C9—C8—C7—C4	-0.7 (9)	Br1—C1—C2—C3	-179.5 (4)
N1—C8—C7—C4	-179.7 (4)	C4—C3—C2—C1	-0.6 (8)
C6—C5—C4—C3	-1.8 (7)	C2—C1—C6—C5	-0.2 (8)
C6—C5—C4—C7	-179.8 (4)	Br1—C1—C6—C5	179.2 (4)
C8—C7—C4—C3	8.7 (8)	C4—C5—C6—C1	1.1 (8)

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