N-(2-Acetylphenyl)benzenesulfonamide

R. R. Saravanan,[a] V. Dhayalan,[b] A. K. Mohanakrishnan,[b] G. Chakkaravarthi[c] and V. Manivannan[d]*

[a]Department of Physics, PRIST University, Thanjavur 614 904, Tamil Nadu, India, [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, [c]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India, and [d]Department of Research and Development, PRIST University, Vallam, Thanjavur 613 403, Tamil Nadu, India
Correspondence e-mail: manivan_1999@yahoo.com

In the title compound, $C_{14}H_{13}NO_3S$, the phenyl ring makes a dihedral angle of 81.5 (1)° with the benzene ring. The molecular structure is stabilized by an intramolecular N—H···O hydrogen bond and weak C—H···O interactions. In the crystal structure, molecules are linked by weak intermolecular C—H···O and C—H···π interactions.

Related literature

For the biological activity of benzenesulfonamide derivatives, see: Badr (2008); Hanafy *et al.* (2007); Yang *et al.* (2002). For related structures, see: Chakkaravarthi *et al.* (2007); Li & Yang (2006). For graph-set notation, see: Bernstein *et al.* (1995).
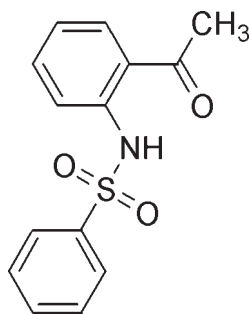
Experimental

Crystal data

$C_{14}H_{13}NO_3S$	a = 7.9909 (3) Å
M_r = 275.31	b = 8.6860 (4) Å
Triclinic, $P\bar{1}$	c = 10.0701 (4) Å
α = 88.016 (2)°	Mo $K\alpha$ radiation
β = 68.673 (3)°	μ = 0.25 mm^{-1}
γ = 83.424 (2)°	T = 295 K
V = 646.79 (5) Å^3	0.24 × 0.20 × 0.20 mm
Z = 2	

Data collection

Bruker Kappa APEX2 diffractometer	18690 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	5104 independent reflections
T_{min} = 0.942, T_{max} = 0.951	3886 reflections with $I > 2\sigma(I)$
	R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045	173 parameters
$wR(F^2)$ = 0.142	H-atom parameters constrained
S = 1.03	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
5104 reflections	$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.86	2.03	2.596 (2)	123
C2—H2···O1	0.93	2.52	2.893 (2)	104
C12—H12···O1	0.93	2.40	3.057 (2)	128
C11—H11···O1^i	0.93	2.51	3.380 (2)	156
C14—H14C···$Cg1^{ii}$	0.96	2.96	3.763 (2)	142

Symmetry codes: (i) $-x, -y + 2, -z$; (ii) $-x + 1, -y + 1, -z$. $Cg1$ is the centroid of the benzene C7–C12 ring.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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supporting information

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S1. Comment

The benzenesulfonamide derivatives are known to exhibit antitumor (Yang *et al.*, 2002), anti-bacterial (Badr, 2008) and anti-fungal (Hanafy *et al.*, 2007) activities. The geometric parameters in (I) (Fig. 1) agree with the reported values of similar structures (Chakkaravarthi *et al.*, 2007; Li & Yang, 2006).

The phenyl ring C1—C6 makes the dihedral angle of 81.5 (1)° with the benzene ring C7—C12. A distorted tetrahedral geometry [O1—S1—N1 109.49 (6)° and O2—S1—N1 104.32 (6)°] is observed around the S1 atom. The molecular structure is stabilized by weak intramolecular C—H···O and N—H···O interactions and the molecules are linked by weak intermolecular C—H···O and C—H···π interactions (Fig. 2 & Table 1). The intramolecular N1—H1···O3 interaction generates a six-membered ring, with graph-set motif S(6) and the intermolecular C11—H11···O1 interaction generates a fourteen membered ring, with graph-set motif $R_2^2(14)$.

S2. Experimental

To a stirred solution of 1-(2-aminophenyl)ethanone (3.0 g, 22.19 mmol) in dry DCM (50 ml) at room temperature, pyridine (1.75 g, 22.12 mmol) was slowly added. After 10 min, PhSO$_2$Cl (4.71 g, 26.61 mmol) was added and stirred at room temperature for 15 h. Then the reaction mixture was poured over crushed ice containing conc. HCl (10 ml), work up of the reaction followed by recrystallization from CDCl$_3$ gave the compound.

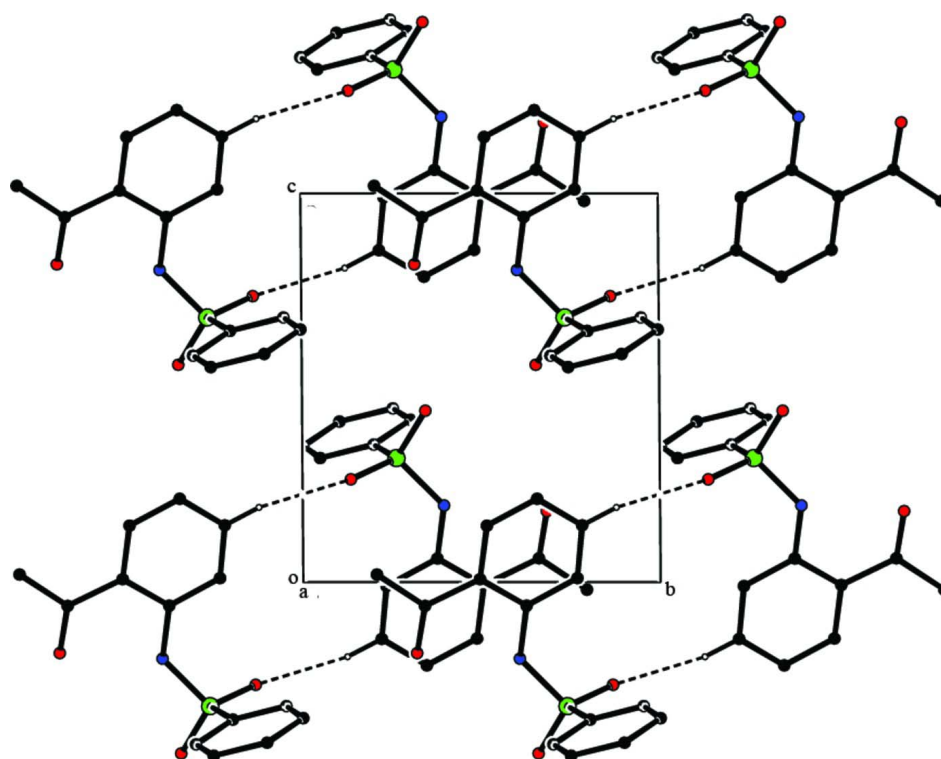### S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C) for N—H, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH$_3$.
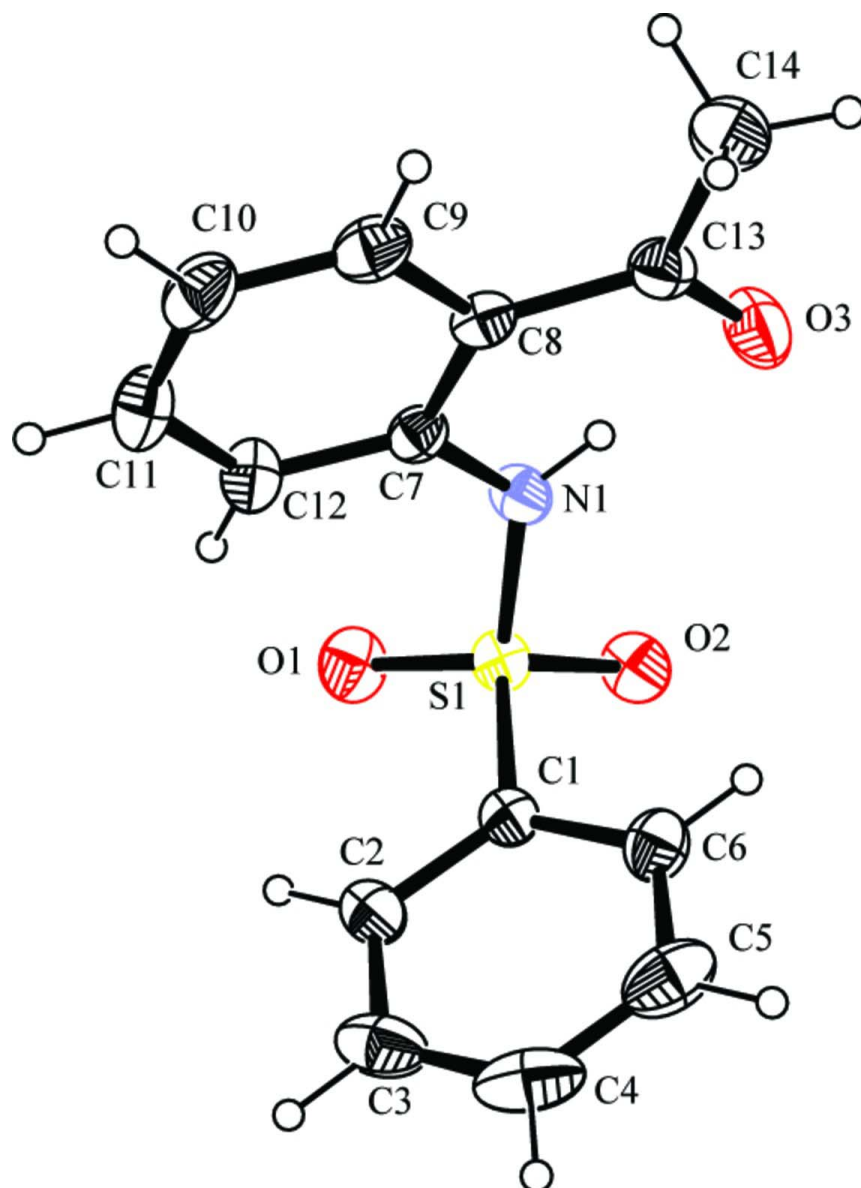
Figure 1
The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

Figure 2

The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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$C_{14}H_{13}NO_3S$	$Z = 2$
$M_r = 275.31$	$F(000) = 288$
Triclinic, $P\bar{1}$	$D_x = 1.414$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.9909$ (3) Å	Cell parameters from 8349 reflections
$b = 8.6860$ (4) Å	$\theta = 2.2–33.4°$
$c = 10.0701$ (4) Å	$\mu = 0.25$ mm^{-1}
$\alpha = 88.016$ (2)°	$T = 295$ K
$\beta = 68.673$ (3)°	Block, colourless
$\gamma = 83.424$ (2)°	$0.24 \times 0.20 \times 0.20$ mm
$V = 646.79$ (5) Å^3	

Data collection

Bruker Kappa APEX2 diffractometer	18690 measured reflections
Radiation source: fine-focus sealed tube	5104 independent reflections
Graphite monochromator	3886 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{int} = 0.023$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 33.6°$, $\theta_{min} = 2.2°$
$T_{min} = 0.942$, $T_{max} = 0.951$	$h = -12\rightarrow12$
	$k = -13\rightarrow13$
	$l = -15\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.142$	
$S = 1.03$	H-atom parameters constrained
5104 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.0784P]$
173 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.35$ e Å^{-3}
	$\Delta\rho_{min} = -0.41$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
S1	0.21195 (4)	0.73664 (3)	−0.31916 (3)	0.04029 (10)
O1	0.07767 (14)	0.86458 (13)	−0.26435 (13)	0.0585 (3)
O2	0.21545 (16)	0.65492 (13)	−0.44094 (11)	0.0551 (3)
O3	0.3126 (2)	0.31720 (13)	−0.18266 (13)	0.0665 (3)
N1	0.18906 (16)	0.60455 (13)	−0.19706 (11)	0.0434 (2)
H1	0.1726	0.5138	−0.2181	0.052*
C1	0.42453 (17)	0.80008 (14)	−0.35373 (12)	0.0382 (2)
C2	0.4361 (2)	0.95013 (16)	−0.31914 (15)	0.0486 (3)
H2	0.3324	1.0179	−0.2762	0.058*
C3	0.6061 (3)	0.9970 (2)	−0.35014 (18)	0.0661 (5)
H3	0.6175	1.0975	−0.3282	0.079*
C4	0.7578 (3)	0.8955 (3)	−0.4131 (2)	0.0755 (6)
H4	0.8714	0.9279	−0.4334	0.091*
C5	0.7442 (2)	0.7457 (3)	−0.4469 (2)	0.0717 (5)
H5	0.8481	0.6780	−0.4893	0.086*
C6	0.5762 (2)	0.69662 (19)	−0.41754 (16)	0.0528 (3)
H6	0.5653	0.5963	−0.4401	0.063*
C7	0.19359 (15)	0.62435 (14)	−0.06059 (12)	0.0378 (2)
C8	0.24861 (16)	0.49460 (15)	0.00745 (12)	0.0396 (2)
C9	0.2463 (2)	0.51504 (19)	0.14513 (14)	0.0522 (3)
H9	0.2818	0.4304	0.1916	0.063*
C10	0.1932 (2)	0.6560 (2)	0.21426 (16)	0.0603 (4)
H10	0.1927	0.6662	0.3060	0.072*
C11	0.1410 (2)	0.7816 (2)	0.14616 (17)	0.0626 (4)
H11	0.1061	0.8776	0.1920	0.075*
C12	0.1396 (2)	0.76713 (18)	0.01025 (16)	0.0523 (3)
H12	0.1025	0.8529	−0.0341	0.063*
C13	0.30558 (19)	0.34007 (16)	−0.06119 (15)	0.0468 (3)
C14	0.3558 (3)	0.2063 (2)	0.0194 (2)	0.0679 (5)
H14A	0.3861	0.1139	−0.0380	0.102*
H14B	0.2557	0.1924	0.1059	0.102*
H14C	0.4581	0.2265	0.0420	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.04233 (17)	0.04223 (16)	0.04242 (17)	−0.00101 (11)	−0.02377 (13)	0.00144 (11)
O1	0.0481 (5)	0.0583 (6)	0.0696 (7)	0.0125 (4)	−0.0272 (5)	0.0008 (5)
O2	0.0710 (7)	0.0605 (6)	0.0490 (5)	−0.0116 (5)	−0.0384 (5)	0.0009 (4)
O3	0.1044 (10)	0.0446 (5)	0.0568 (6)	−0.0009 (6)	−0.0384 (6)	−0.0043 (4)
N1	0.0550 (6)	0.0410 (5)	0.0411 (5)	−0.0103 (4)	−0.0243 (5)	0.0022 (4)
C1	0.0429 (6)	0.0398 (5)	0.0355 (5)	−0.0036 (4)	−0.0189 (4)	0.0031 (4)
C2	0.0650 (8)	0.0437 (6)	0.0444 (6)	−0.0105 (6)	−0.0276 (6)	0.0039 (5)
C3	0.0859 (12)	0.0725 (10)	0.0590 (9)	−0.0414 (10)	−0.0410 (9)	0.0211 (8)
C4	0.0614 (10)	0.1176 (17)	0.0625 (10)	−0.0449 (11)	−0.0334 (8)	0.0380 (11)
C5	0.0411 (7)	0.1059 (15)	0.0622 (10)	−0.0024 (8)	−0.0149 (7)	0.0170 (10)
C6	0.0467 (7)	0.0562 (8)	0.0530 (7)	0.0033 (6)	−0.0174 (6)	−0.0028 (6)
C7	0.0331 (5)	0.0453 (6)	0.0352 (5)	−0.0070 (4)	−0.0118 (4)	0.0001 (4)
C8	0.0355 (5)	0.0482 (6)	0.0352 (5)	−0.0092 (4)	−0.0119 (4)	0.0043 (4)
C9	0.0548 (8)	0.0672 (9)	0.0376 (6)	−0.0123 (7)	−0.0193 (5)	0.0081 (6)
C10	0.0634 (9)	0.0818 (11)	0.0365 (6)	−0.0114 (8)	−0.0174 (6)	−0.0065 (7)
C11	0.0681 (10)	0.0686 (10)	0.0477 (8)	0.0010 (8)	−0.0175 (7)	−0.0198 (7)
C12	0.0559 (8)	0.0520 (7)	0.0486 (7)	0.0032 (6)	−0.0202 (6)	−0.0078 (6)
C13	0.0494 (7)	0.0433 (6)	0.0473 (7)	−0.0069 (5)	−0.0171 (5)	0.0061 (5)
C14	0.0797 (12)	0.0559 (9)	0.0628 (10)	0.0037 (8)	−0.0240 (8)	0.0138 (7)

Geometric parameters (Å, º)

S1—O1	1.4246 (11)	C6—H6	0.9300
S1—O2	1.4280 (10)	C7—C12	1.3957 (19)
S1—N1	1.6274 (11)	C7—C8	1.4090 (17)
S1—C1	1.7555 (13)	C8—C9	1.3969 (17)
O3—C13	1.2260 (17)	C8—C13	1.4772 (19)
N1—C7	1.4049 (15)	C9—C10	1.374 (2)
N1—H1	0.8597	C9—H9	0.9300
C1—C2	1.3824 (18)	C10—C11	1.374 (3)
C1—C6	1.3834 (19)	C10—H10	0.9300
C2—C3	1.385 (2)	C11—C12	1.383 (2)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.373 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.495 (2)
C4—C5	1.382 (3)	C14—H14A	0.9600
C4—H4	0.9300	C14—H14B	0.9600
C5—C6	1.380 (2)	C14—H14C	0.9600
C5—H5	0.9300		
O1—S1—O2	118.85 (7)	C12—C7—N1	121.74 (12)
O1—S1—N1	109.49 (6)	C12—C7—C8	119.64 (12)
O2—S1—N1	104.32 (6)	N1—C7—C8	118.58 (11)
O1—S1—C1	108.17 (7)	C9—C8—C7	117.87 (12)
O2—S1—C1	109.31 (6)	C9—C8—C13	119.87 (12)

N1—S1—C1	105.96 (6)	C7—C8—C13	122.26 (11)
C7—N1—S1	126.34 (9)	C10—C9—C8	122.23 (14)
C7—N1—H1	116.8	C10—C9—H9	118.9
S1—N1—H1	116.8	C8—C9—H9	118.9
C2—C1—C6	122.22 (13)	C11—C10—C9	119.21 (14)
C2—C1—S1	119.85 (11)	C11—C10—H10	120.4
C6—C1—S1	117.93 (10)	C9—C10—H10	120.4
C1—C2—C3	118.27 (15)	C10—C11—C12	120.77 (15)
C1—C2—H2	120.9	C10—C11—H11	119.6
C3—C2—H2	120.9	C12—C11—H11	119.6
C4—C3—C2	120.15 (16)	C11—C12—C7	120.27 (15)
C4—C3—H3	119.9	C11—C12—H12	119.9
C2—C3—H3	119.9	C7—C12—H12	119.9
C3—C4—C5	120.96 (15)	O3—C13—C8	122.15 (12)
C3—C4—H4	119.5	O3—C13—C14	118.48 (14)
C5—C4—H4	119.5	C8—C13—C14	119.37 (13)
C6—C5—C4	119.90 (18)	C13—C14—H14A	109.5
C6—C5—H5	120.0	C13—C14—H14B	109.5
C4—C5—H5	120.0	H14A—C14—H14B	109.5
C5—C6—C1	118.50 (16)	C13—C14—H14C	109.5
C5—C6—H6	120.7	H14A—C14—H14C	109.5
C1—C6—H6	120.7	H14B—C14—H14C	109.5
O1—S1—N1—C7	−57.47 (12)	S1—N1—C7—C12	29.02 (17)
O2—S1—N1—C7	174.32 (11)	S1—N1—C7—C8	−153.13 (10)
C1—S1—N1—C7	58.98 (12)	C12—C7—C8—C9	0.11 (18)
O1—S1—C1—C2	3.58 (12)	N1—C7—C8—C9	−177.78 (11)
O2—S1—C1—C2	134.36 (10)	C12—C7—C8—C13	179.40 (12)
N1—S1—C1—C2	−113.75 (10)	N1—C7—C8—C13	1.50 (17)
O1—S1—C1—C6	−175.46 (10)	C7—C8—C9—C10	−0.2 (2)
O2—S1—C1—C6	−44.68 (12)	C13—C8—C9—C10	−179.52 (14)
N1—S1—C1—C6	67.21 (11)	C8—C9—C10—C11	−0.2 (2)
C6—C1—C2—C3	0.07 (19)	C9—C10—C11—C12	0.7 (3)
S1—C1—C2—C3	−178.93 (10)	C10—C11—C12—C7	−0.8 (3)
C1—C2—C3—C4	−0.2 (2)	N1—C7—C12—C11	178.19 (13)
C2—C3—C4—C5	0.1 (2)	C8—C7—C12—C11	0.4 (2)
C3—C4—C5—C6	0.2 (3)	C9—C8—C13—O3	−178.77 (14)
C4—C5—C6—C1	−0.3 (2)	C7—C8—C13—O3	2.0 (2)
C2—C1—C6—C5	0.2 (2)	C9—C8—C13—C14	1.5 (2)
S1—C1—C6—C5	179.21 (12)	C7—C8—C13—C14	−177.78 (14)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.86	2.03	2.596 (2)	123
C2—H2···O1	0.93	2.52	2.893 (2)	104
C12—H12···O1	0.93	2.40	3.057 (2)	128

C11—H11···O1[i]	0.93	2.51	3.380 (2)	156
C14—H14*C*···*Cg*1[ii]	0.96	2.96	3.763 (2)	142

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