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## Structure Reports

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## 2-(Benzenesulfonamido)pyridinium perchlorate

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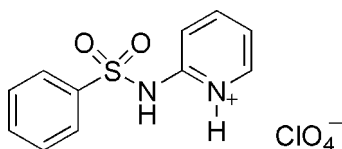
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Key indicators: single-crystal X-ray study;  $T = 113$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.092; data-to-parameter ratio = 15.4.

In the title compound,  $\text{C}_{11}\text{H}_{11}\text{N}_2\text{O}_2\text{S}^+\cdot\text{ClO}_4^-$ , the dihedral angle between the benzene and pyridinium rings is  $87.33$  ( $10$ )°. An intramolecular  $\text{N}-\text{H}\cdots\text{O}$  interaction, with an  $\text{S}=\text{O}$ -bonded O atom as receptor, occurs in the cation. In the crystal structure, ion pairs occur, being linked by strong  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds. The perchlorate anion plays a further role in the molecular packing by accepting several weak  $\text{C}-\text{H}\cdots\text{O}$  interactions.

## Related literature

For the synthesis, see: Li, Yang *et al.* (2008). For a related structure containing the same cation, see: Li & Li (2009). For related structures, see: Li *et al.* (2008*a,b*). For applications of pyridinium salts, see: Li *et al.* (2007); Li, Fan *et al.* (2008); Miyashita *et al.* (1977); Ganeshpure *et al.* (2007).



## Experimental

## Crystal data

$\text{C}_{11}\text{H}_{11}\text{N}_2\text{O}_2\text{S}^+\cdot\text{ClO}_4^-$   
 $M_r = 334.73$   
 Triclinic,  $P\bar{1}$   
 $a = 5.6594$  (11) Å

$b = 7.5996$  (15) Å  
 $c = 16.157$  (3) Å  
 $\alpha = 83.21$  (3)°  
 $\beta = 83.70$  (3)°

$\gamma = 73.84$  (3)°  
 $V = 660.6$  (2) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation

$\mu = 0.48$  mm<sup>-1</sup>  
 $T = 113$  K  
 $0.20 \times 0.10 \times 0.08$  mm

## Data collection

Rigaku Saturn CCD diffractometer  
 Absorption correction: multi-scan  
 (*CrystalClear*; Rigaku/MS, 2005)  
 $T_{\min} = 0.911$ ,  $T_{\max} = 0.963$

5339 measured reflections  
 3051 independent reflections  
 2473 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.092$   
 $S = 1.07$   
 3051 reflections  
 198 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.42$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O1}$	0.82 (2)	2.01 (2)	2.694 (2)	141 (2)
$\text{N2}-\text{H2A}\cdots\text{O4}$	0.81 (2)	2.02 (2)	2.808 (2)	165 (2)
$\text{C1}-\text{H1}\cdots\text{O3}^{\text{ii}}$	0.95	2.37	3.301 (3)	166
$\text{C3}-\text{H3}\cdots\text{O5}^{\text{ii}}$	0.95	2.44	3.303 (3)	151
$\text{C7}-\text{H7}\cdots\text{O4}^{\text{iii}}$	0.95	2.53	3.417 (2)	156
$\text{C8}-\text{H8}\cdots\text{O3}^{\text{iii}}$	0.95	2.58	3.251 (3)	128

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

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku/MS, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2972).

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## supporting information

*Acta Cryst.* (2009). E65, o1430 [doi:10.1107/S1600536809019205]

**2-(Benzenesulfonamido)pyridinium perchlorate**

Xun Li, Dan Xie, Zhi-Hong Xiao and Chang-Zhu Li

**S1. Comment**

Organic pyridinium salts have been used as not only supramolecular guests (Li *et al.*, 2007; Li, Fan, Fan *et al.*, 2008), but also catalysts and/or media for esterification (Ganeshpure *et al.* 2007; Miyashita *et al.* 1977). To seek a new pyridinium catalyst for biodiesel transformation, the title compound, (I), was synthesized and further determined by X-ray diffraction.

The title compound, (I), consists of a pyridinium cation and a perchlorate anion (Fig. 1). In the cation, the distance [1.383 (2) Å] between the pyridinium C atom and its connected amino N atom is slightly longer than the nitrate [1.378 (2) Å] (Li *et al.* 2009), also showing some conjugation of amino group with pyridinium ring. The benzene ring constructs an angle of 87.33 (10)° with the pyridinium ring, similar to the nitrate [87.59 (8)°]. The cation structure is stabilized by an intramolecular N—H···O hydrogen bond (Table 1), with S=O oxygen as H-bonding receptor, different from by C—H···O interaction in the nitrate.

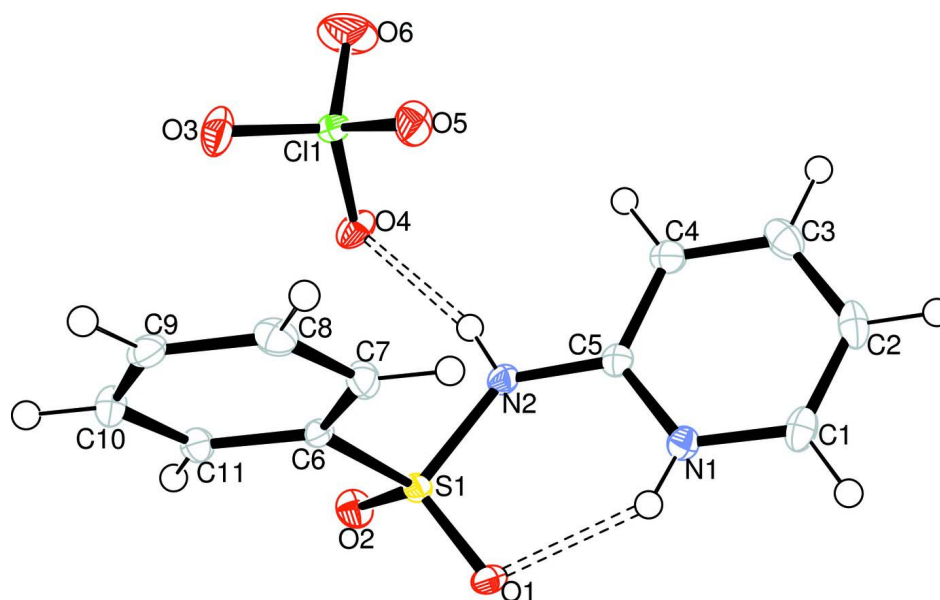
Like the nitrate, in the crystal structure, a strong N—H···O hydrogen bond link the cation and anion (Table 1). The anion ClO<sub>4</sub> plays a great important role in the molecular packing *via* weak C—H···O interactions (Table 1).

**S2. Experimental**

The title compound was prepared according to the reported literature (Li, Yang *et al.* 2008). Colourless needles of (I) were obtained by evaporation of a perchloric acid solution of the sulfonamide.

**S3. Refinement**

The H atoms bound to C were positioned geometrically (C—H = 0.95 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ . The N—H hydrogen atoms were refined with their isotropic displacement parameters, and N—H distances are restrained to 0.82 (2) and 0.81 (2) Å, respectively.

**Figure 1**

View of the molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level and H atoms shown as small spheres of arbitrary radius. Dashed lines indicate hydrogen bonds.

## 2-(Benzenesulfonamido)pyridinium perchlorate

### Crystal data

$C_{11}H_{11}N_2O_2S^+ \cdot ClO_4^-$

$M_r = 334.73$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 5.6594$  (11) Å

$b = 7.5996$  (15) Å

$c = 16.157$  (3) Å

$\alpha = 83.21$  (3)°

$\beta = 83.70$  (3)°

$\gamma = 73.84$  (3)°

$V = 660.6$  (2) Å<sup>3</sup>

$Z = 2$

$F(000) = 344$

$D_x = 1.683$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2172 reflections

$\theta = 2.8$ – $27.9$ °

$\mu = 0.48$  mm<sup>-1</sup>

$T = 113$  K

Needle, colourless

$0.20 \times 0.10 \times 0.08$  mm

### Data collection

Rigaku Saturn CCD  
diffractometer

Radiation source: rotating anode

Confocal monochromator

Detector resolution: 7.31 pixels mm<sup>-1</sup>

$\omega$  and  $\phi$  scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku/MSK, 2005)

$T_{\min} = 0.911$ ,  $T_{\max} = 0.963$

5339 measured reflections

3051 independent reflections

2473 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.9$ °,  $\theta_{\min} = 2.8$ °

$h = -7 \rightarrow 7$

$k = -7 \rightarrow 9$

$l = -19 \rightarrow 21$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.092$   
 $S = 1.07$   
 3051 reflections  
 198 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 atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.3333P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.32 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.42 \text{ e } \text{Å}^{-3}$

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 ( $\text{Å}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.22811 (8)	0.24398 (6)	0.16564 (3)	0.01285 (12)
O1	0.3752 (3)	0.36817 (19)	0.13565 (8)	0.0188 (3)
O2	-0.0260 (2)	0.2927 (2)	0.14890 (8)	0.0195 (3)
N1	0.5339 (3)	0.3703 (2)	0.28668 (10)	0.0146 (3)
N2	0.2351 (3)	0.2162 (2)	0.26820 (9)	0.0142 (3)
C1	0.6774 (3)	0.4261 (3)	0.33434 (12)	0.0178 (4)
H1	0.7775	0.5030	0.3096	0.021*
C2	0.6782 (4)	0.3717 (3)	0.41768 (12)	0.0202 (4)
H2	0.7815	0.4072	0.4513	0.024*
C3	0.5244 (4)	0.2628 (3)	0.45284 (12)	0.0214 (4)
H3	0.5208	0.2255	0.5111	0.026*
C4	0.3781 (4)	0.2091 (3)	0.40365 (11)	0.0167 (4)
H4	0.2729	0.1353	0.4276	0.020*
C5	0.3861 (3)	0.2644 (3)	0.31822 (11)	0.0133 (4)
C6	0.3713 (3)	0.0251 (2)	0.13242 (11)	0.0122 (3)
C7	0.6069 (3)	-0.0679 (3)	0.15558 (11)	0.0167 (4)
H7	0.6874	-0.0172	0.1915	0.020*
C8	0.7216 (4)	-0.2369 (3)	0.12480 (11)	0.0185 (4)
H8	0.8823	-0.3031	0.1397	0.022*
C9	0.6018 (4)	-0.3089 (3)	0.07244 (12)	0.0179 (4)
H9	0.6818	-0.4241	0.0514	0.021*
C10	0.3665 (4)	-0.2150 (3)	0.05020 (12)	0.0193 (4)
H10	0.2865	-0.2659	0.0142	0.023*
C11	0.2487 (3)	-0.0472 (3)	0.08060 (11)	0.0157 (4)

H11	0.0869	0.0175	0.0663	0.019*
H1A	0.536 (4)	0.398 (3)	0.2358 (15)	0.022 (6)*
H2A	0.152 (4)	0.150 (3)	0.2905 (14)	0.019 (6)*
C11	0.06395 (8)	-0.20083 (6)	0.34300 (3)	0.01538 (12)
O3	0.0680 (3)	-0.3209 (2)	0.28027 (10)	0.0267 (3)
O4	-0.0763 (2)	-0.01507 (19)	0.31513 (9)	0.0209 (3)
O5	0.3112 (3)	-0.1954 (2)	0.35352 (9)	0.0243 (3)
O6	-0.0508 (3)	-0.2619 (3)	0.42029 (10)	0.0415 (5)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0155 (2)	0.0101 (2)	0.0123 (2)	-0.00192 (17)	-0.00278 (15)	-0.00055 (15)
O1	0.0296 (8)	0.0140 (7)	0.0144 (6)	-0.0102 (6)	-0.0003 (5)	0.0011 (5)
O2	0.0169 (7)	0.0168 (7)	0.0220 (7)	0.0020 (6)	-0.0067 (5)	-0.0018 (5)
N1	0.0152 (8)	0.0138 (8)	0.0152 (8)	-0.0041 (6)	-0.0009 (6)	-0.0024 (6)
N2	0.0156 (8)	0.0148 (8)	0.0139 (7)	-0.0075 (7)	0.0006 (6)	-0.0008 (6)
C1	0.0127 (9)	0.0145 (10)	0.0268 (10)	-0.0023 (7)	-0.0014 (7)	-0.0081 (8)
C2	0.0169 (9)	0.0203 (10)	0.0245 (10)	-0.0014 (8)	-0.0065 (7)	-0.0104 (8)
C3	0.0230 (10)	0.0221 (11)	0.0165 (9)	0.0006 (9)	-0.0036 (7)	-0.0052 (8)
C4	0.0190 (9)	0.0148 (10)	0.0152 (8)	-0.0032 (8)	0.0002 (7)	-0.0017 (7)
C5	0.0122 (8)	0.0097 (9)	0.0166 (8)	0.0003 (7)	-0.0012 (6)	-0.0029 (7)
C6	0.0149 (9)	0.0099 (9)	0.0119 (8)	-0.0035 (7)	-0.0007 (6)	-0.0004 (6)
C7	0.0171 (9)	0.0160 (10)	0.0173 (9)	-0.0032 (8)	-0.0056 (7)	-0.0020 (7)
C8	0.0179 (9)	0.0169 (10)	0.0170 (9)	0.0010 (8)	-0.0017 (7)	-0.0002 (7)
C9	0.0246 (10)	0.0108 (9)	0.0171 (9)	-0.0043 (8)	0.0017 (7)	-0.0009 (7)
C10	0.0241 (10)	0.0181 (10)	0.0187 (9)	-0.0088 (8)	-0.0029 (7)	-0.0049 (7)
C11	0.0152 (9)	0.0167 (10)	0.0159 (8)	-0.0051 (8)	-0.0032 (7)	-0.0005 (7)
Cl1	0.0175 (2)	0.0130 (2)	0.0159 (2)	-0.00511 (18)	-0.00268 (16)	0.00102 (16)
O3	0.0278 (8)	0.0179 (8)	0.0367 (8)	-0.0036 (7)	-0.0096 (6)	-0.0113 (6)
O4	0.0163 (7)	0.0104 (7)	0.0344 (8)	-0.0002 (6)	-0.0049 (6)	-0.0012 (6)
O5	0.0179 (7)	0.0235 (8)	0.0331 (8)	-0.0049 (6)	-0.0116 (6)	-0.0018 (6)
O6	0.0476 (11)	0.0515 (12)	0.0251 (8)	-0.0225 (10)	0.0047 (7)	0.0133 (8)

*Geometric parameters (Å, °)*

S1—O2	1.4296 (14)	C4—H4	0.9500
S1—O1	1.4352 (15)	C6—C11	1.391 (3)
S1—N2	1.6488 (16)	C6—C7	1.393 (3)
S1—C6	1.7540 (19)	C7—C8	1.391 (3)
N1—C5	1.338 (2)	C7—H7	0.9500
N1—C1	1.356 (2)	C8—C9	1.384 (3)
N1—H1A	0.82 (2)	C8—H8	0.9500
N2—C5	1.383 (2)	C9—C10	1.388 (3)
N2—H2A	0.81 (2)	C9—H9	0.9500
C1—C2	1.361 (3)	C10—C11	1.384 (3)
C1—H1	0.9500	C10—H10	0.9500
C2—C3	1.395 (3)	C11—H11	0.9500

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C2—H2	0.9500	C11—O6	1.4315 (16)
C3—C4	1.376 (3)	C11—O3	1.4358 (15)
C3—H3	0.9500	C11—O5	1.4403 (15)
C4—C5	1.394 (2)	C11—O4	1.4594 (15)
O2—S1—O1	119.45 (9)	N2—C5—C4	119.97 (17)
O2—S1—N2	106.71 (9)	C11—C6—C7	121.88 (18)
O1—S1—N2	106.24 (9)	C11—C6—S1	118.51 (14)
O2—S1—C6	108.52 (9)	C7—C6—S1	119.56 (14)
O1—S1—C6	110.07 (9)	C8—C7—C6	118.41 (18)
N2—S1—C6	104.81 (9)	C8—C7—H7	120.8
C5—N1—C1	122.75 (17)	C6—C7—H7	120.8
C5—N1—H1A	116.0 (17)	C9—C8—C7	120.05 (18)
C1—N1—H1A	121.3 (17)	C9—C8—H8	120.0
C5—N2—S1	129.79 (14)	C7—C8—H8	120.0
C5—N2—H2A	116.6 (16)	C8—C9—C10	120.91 (19)
S1—N2—H2A	112.8 (16)	C8—C9—H9	119.5
N1—C1—C2	119.98 (19)	C10—C9—H9	119.5
N1—C1—H1	120.0	C11—C10—C9	119.91 (18)
C2—C1—H1	120.0	C11—C10—H10	120.0
C1—C2—C3	118.80 (18)	C9—C10—H10	120.0
C1—C2—H2	120.6	C10—C11—C6	118.83 (18)
C3—C2—H2	120.6	C10—C11—H11	120.6
C4—C3—C2	120.39 (18)	C6—C11—H11	120.6
C4—C3—H3	119.8	O6—C11—O3	109.89 (11)
C2—C3—H3	119.8	O6—C11—O5	110.65 (10)
C3—C4—C5	119.16 (19)	O3—C11—O5	110.12 (10)
C3—C4—H4	120.4	O6—C11—O4	109.52 (11)
C5—C4—H4	120.4	O3—C11—O4	108.72 (9)
N1—C5—N2	121.08 (16)	O5—C11—O4	107.89 (9)
N1—C5—C4	118.89 (17)		
O2—S1—N2—C5	-141.28 (17)	O1—S1—C6—C11	-118.07 (15)
O1—S1—N2—C5	-12.81 (19)	N2—S1—C6—C11	128.06 (15)
C6—S1—N2—C5	103.73 (18)	O2—S1—C6—C7	-168.22 (15)
C5—N1—C1—C2	1.1 (3)	O1—S1—C6—C7	59.37 (17)
N1—C1—C2—C3	-1.7 (3)	N2—S1—C6—C7	-54.50 (17)
C1—C2—C3—C4	1.1 (3)	C11—C6—C7—C8	0.7 (3)
C2—C3—C4—C5	0.2 (3)	S1—C6—C7—C8	-176.66 (14)
C1—N1—C5—N2	177.48 (17)	C6—C7—C8—C9	0.0 (3)
C1—N1—C5—C4	0.2 (3)	C7—C8—C9—C10	-0.3 (3)
S1—N2—C5—N1	9.9 (3)	C8—C9—C10—C11	-0.1 (3)
S1—N2—C5—C4	-172.85 (14)	C9—C10—C11—C6	0.8 (3)
C3—C4—C5—N1	-0.8 (3)	C7—C6—C11—C10	-1.1 (3)
C3—C4—C5—N2	-178.17 (17)	S1—C6—C11—C10	176.28 (14)
O2—S1—C6—C11	14.34 (17)		

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*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1A $\cdots$ O1	0.82 (2)	2.01 (2)	2.694 (2)	141 (2)
N2—H2A $\cdots$ O4	0.81 (2)	2.02 (2)	2.808 (2)	165 (2)
C1—H1 $\cdots$ O3 <sup>i</sup>	0.95	2.37	3.301 (3)	166
C3—H3 $\cdots$ O5 <sup>ii</sup>	0.95	2.44	3.303 (3)	151
C7—H7 $\cdots$ O4 <sup>iii</sup>	0.95	2.53	3.417 (2)	156
C8—H8 $\cdots$ O3 <sup>iii</sup>	0.95	2.58	3.251 (3)	128

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