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# 2-(1,3-Thiazol-4-yl)benzimidazolium nitrate monohydrate

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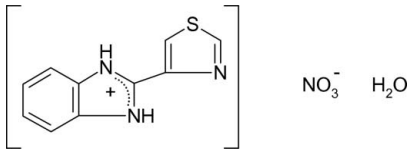
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.100; data-to-parameter ratio = 13.2.

In the title compound, $C_{10}H_8N_3S^+\cdot NO_3^-\cdot H_2O$, one of the N atoms of the benzimidazole unit is protonated, unlike than that in the thiazole group. This protonation leads to equalization of the bond angles at the two N atoms of the benzimidazole group. The benzimidazole and thiazole systems are almost coplanar, forming a dihedral angle of 0.5 (2)°. In the crystal, the nitrate anion and water molecule bridge the thiabendazolium cations through N—H···O and O—H···O hydrogen bonds, leading to a supramolecular network based on an infinite one-dimensional chain using [001] as base vector.

## Related literature

For the antiviral action and anthelmintic activity of substituted benzimidazoles, see: Goodgame *et al.* (1985). Related structures have been reported: thiabendazole (Trus & Marsh, 1973); thiabendazolium nitrate (Murugesan *et al.*, 1998; Devereux *et al.*, 2004); thiabendazolium perchlorate (Stanley *et al.*, 2002); thiabendazolium halide dihydrates (Prabakaran *et al.*, 2000). For structures of transition metal complexes bearing thiabendazole as ligand, see: Kowala & Wunderlich (1973); Udupa & Krebs (1979); Rong *et al.* (1991).




## Experimental

### Crystal data

$C_{10}H_8N_3S^+\cdot NO_3^-\cdot H_2O$
$M_r$ = 282.28
Monoclinic, $P2_1/c$
$a$ = 7.6140 (3) Å
$b$ = 16.3130 (5) Å
$c$ = 10.0990 (3) Å
$\beta$ = 102.731 (4)°
$V$ = 1223.53 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 298 K
0.54 × 0.39 × 0.26 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with an Atlas (Gemini Mo) detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.920, $T_{max}$ = 0.952
5590 measured reflections
2426 independent reflections
1859 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
$S$ = 1.08
2426 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H2$D$···O17 | 0.85 (2) | 2.06 (2) | 2.903 (2) | 168 (2) |
| O1$W$—H1$D$···O16$^{i}$ | 0.78 (2) | 2.24 (3) | 2.969 (2) | 156 (2) |
| N1—H1$N$···O1$W^{i}$ | 0.85 (2) | 1.91 (2) | 2.748 (2) | 168.5 (18) |
| N3—H3$N$···O16$^{ii}$ | 0.82 (2) | 2.58 (2) | 3.300 (2) | 147.5 (18) |
| N3—H3$N$···O17$^{ii}$ | 0.82 (2) | 2.02 (2) | 2.791 (2) | 157 (2) |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2274).

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# supporting information

*Acta Cryst.* (2010). E**66**, o812 [doi:10.1107/S1600536810008433]

## 2-(1,3-Thiazol-4-yl)benzimidazolium nitrate monohydrate

**Marcos Flores-Alamo, Sandra González-Martínez and Silvia E. Castillo-Blum**

### S1. Comment

Substituted benzimidazoles show antiviral action and anthelmintic activity. This has been attributed to their metal-chelating ability (Goodgame *et al.*, 1985). Thiabendazole is a broad-spectrum anthelmintic compound useful in the treatment of human and animal parasitic diseases.

The crystal structures of thiabendazole (Trus & Marsh, 1973), thiabendazolium nitrate (Murugesan *et al.*, 1998; Devereux *et al.*, 2004), thiabendazolium perchlorate (Stanley *et al.*, 2002), thiabendazolium halide dihydrates (Prabakaran *et al.*, 2000), and its complexes with cobalt (Kowala & Wunderlich, 1973), copper (Udupa & Krebs, 1979) and platinum (Rong *et al.*, 1991) have been reported. The present paper deals with the crystal structure of a protonated thiabendazole moiety, namely, thiabendazolium nitrate hydrate.

The asymmetric unit of the title salt contains one protonated 2-(4-thiazolyl)-1*H*-benzimidazol-1-ium cation, one nitrate anion and one water molecule, shown in Fig. 1. The cation is protonated on the benzimidazole iminic nitrogen atom, resulting in delocalization of the double bond over the N—C—N fragment, with C—N distances of 1.326 (2) and 1.327 (2) Å (Table 1), in contrast to the benzimidazole group in the crystal structure of free thiabendazole, where the two bond lengths are different (Trus & Marsh, 1973).

The C—C bond connecting the two ring systems has a length of 1.445 (2) Å, which is the same bond length, within experimental error, as that in neutral thiabendazole. This value suggests appreciable delocalization across this bond (Prabakaran *et al.*, 2000).

The benzimidazole and thiazole systems are coplanar, the dihedral angle between them is 0.5 (2)°.

The thiabendazole cation is involved in a pair of N—H···O, O—H···O hydrogen bonds [N1···O1w: 2.748 (2) Å and N3···O17: 2.791 (2) Å], while the nitrate anion and water molecule display hydrogen bonding (Table 2), which lead to an infinite one-dimensional chain with base vector [0 0 1].

### S2. Experimental

The reaction mixture of 2-(4-thiazolyl)benzimidazole (0.3686 g, 1.83 mmol) with $[Fe(DMSO)_6]NO_3$ (0.3549 g, 0.5 mmol) in acetonitrile (60 ml) was refluxed for 10 h. It yielded pale-yellow crystals of $(C_{10}H_8N_3S)(NO_3).H_2O$ as a byproduct when the solution was left to stand at room temperature for a couple of days.

### S3. Refinement

H atoms bonded to N and O atoms were located in difference maps and were refined with free coordinates and $U_{iso}$(H) = 1.5$U_{eq}$(N) and 1.2$U_{eq}$(O). H atoms attached to C atoms were placed in geometrically idealized positions and refined as riding on their parent atoms, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

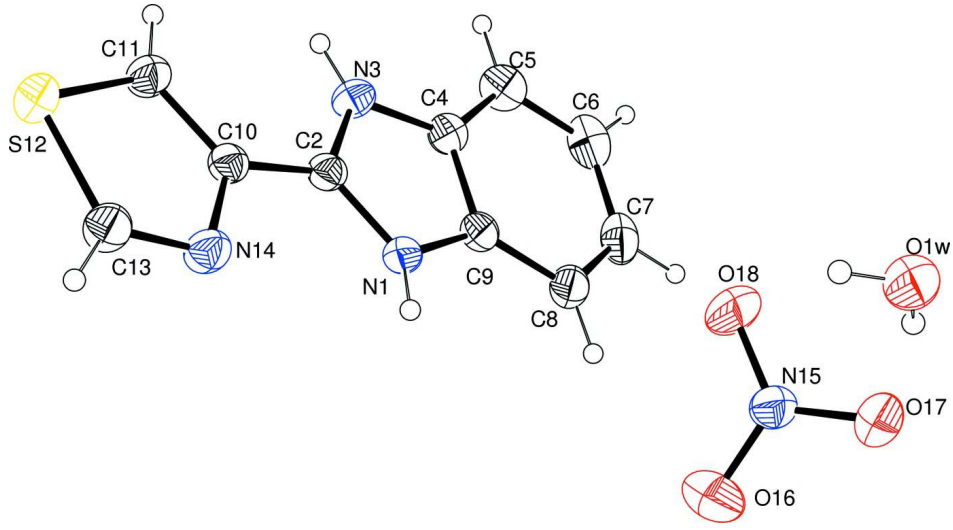


**Figure 1**

The molecular structure of the title salt, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

### 2-(1,3-Thiazol-4-yl)benzimidazolium nitrate monohydrate

*Crystal data*

$C_{10}H_8N_3S^+\cdot NO_3^-\cdot H_2O$
$M_r = 282.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.6140\ (3)$ Å
$b = 16.3130\ (5)$ Å
$c = 10.0990\ (3)$ Å
$\beta = 102.731\ (4)°$
$V = 1223.53\ (7)$ Å$^3$
$Z = 4$
$F(000) = 584$
$D_x = 1.532$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3277 reflections
$\theta = 3.2–26.0°$
$\mu = 0.28$ mm$^{-1}$
$T = 298$ K
Prism, pale yellow
0.54 × 0.39 × 0.26 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer with an Atlas (Gemini Mo) detector
Radiation source: X-ray
Graphite monochromator
Detector resolution: 10.4685 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min} = 0.920$, $T_{max} = 0.952$
5590 measured reflections
2426 independent reflections
1859 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 26.1°$, $\theta_{min} = 3.2°$
$h = -9\rightarrow7$
$k = -19\rightarrow20$
$l = -12\rightarrow10$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.100$
$S = 1.08$
2426 reflections
184 parameters
0 restraints
0 constraints
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

$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.057P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C2 | 0.7417 (2) | −0.01688 (10) | 0.01259 (16) | 0.0385 (4) |
| C4 | 0.8456 (2) | 0.11013 (10) | 0.02130 (18) | 0.0416 (4) |
| C5 | 0.8891 (3) | 0.18937 (11) | −0.0082 (2) | 0.0542 (5) |
| H5 | 0.8578 | 0.2102 | −0.096 | 0.065* |
| C6 | 0.9813 (3) | 0.23603 (12) | 0.0988 (2) | 0.0606 (5) |
| H6 | 1.0132 | 0.2897 | 0.084 | 0.073* |
| C7 | 1.0266 (2) | 0.20260 (12) | 0.2293 (2) | 0.0576 (5) |
| H7 | 1.0923 | 0.2346 | 0.2992 | 0.069* |
| C8 | 0.9784 (2) | 0.12463 (12) | 0.25917 (19) | 0.0517 (5) |
| H8 | 1.0062 | 0.1042 | 0.3473 | 0.062* |
| C9 | 0.8865 (2) | 0.07819 (10) | 0.15118 (16) | 0.0416 (4) |
| C10 | 0.6544 (2) | −0.09278 (9) | −0.03838 (16) | 0.0387 (4) |
| C11 | 0.5761 (2) | −0.10865 (11) | −0.17031 (17) | 0.0467 (4) |
| H11 | 0.5695 | −0.0718 | −0.2415 | 0.056* |
| C13 | 0.5667 (3) | −0.21780 (11) | −0.01579 (18) | 0.0507 (4) |
| H13 | 0.5495 | −0.2667 | 0.027 | 0.061* |
| N1 | 0.81909 (19) | −0.00164 (8) | 0.14122 (14) | 0.0403 (3) |
| N3 | 0.7559 (2) | 0.04857 (9) | −0.06229 (15) | 0.0434 (4) |
| N14 | 0.6484 (2) | −0.15582 (9) | 0.05111 (15) | 0.0487 (4) |
| N15 | 0.6705 (2) | 0.07673 (9) | 0.58671 (15) | 0.0502 (4) |
| O1W | 0.2195 (2) | 0.07887 (10) | 0.62504 (15) | 0.0621 (4) |
| O16 | 0.7817 (3) | 0.02340 (12) | 0.61835 (19) | 0.1061 (7) |
| O17 | 0.6049 (2) | 0.10779 (9) | 0.67836 (14) | 0.0724 (4) |
| O18 | 0.6223 (3) | 0.09795 (10) | 0.47009 (14) | 0.0989 (6) |
| S12 | 0.49270 (6) | −0.20485 (3) | −0.18646 (4) | 0.05076 (18) |
| H2D | 0.329 (3) | 0.0937 (14) | 0.647 (2) | 0.076* |
| H1D | 0.205 (3) | 0.0427 (15) | 0.574 (2) | 0.076* |
| H1N | 0.814 (3) | −0.0313 (12) | 0.210 (2) | 0.061* |
| H3N | 0.722 (3) | 0.0536 (13) | −0.145 (2) | 0.061* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C2 | 0.0382 (9) | 0.0415 (9) | 0.0363 (9) | 0.0061 (7) | 0.0094 (7) | 0.0024 (7) |
| C4 | 0.0385 (9) | 0.0433 (9) | 0.0447 (9) | −0.0003 (7) | 0.0131 (7) | 0.0001 (7) |
| C5 | 0.0536 (11) | 0.0513 (11) | 0.0609 (12) | −0.0058 (8) | 0.0193 (10) | 0.0072 (9) |
| C6 | 0.0486 (11) | 0.0507 (11) | 0.0877 (16) | −0.0080 (9) | 0.0261 (11) | −0.0116 (11) |
| C7 | 0.0421 (10) | 0.0577 (12) | 0.0726 (13) | −0.0018 (8) | 0.0119 (9) | −0.0247 (10) |
| C8 | 0.0462 (10) | 0.0564 (11) | 0.0496 (10) | 0.0067 (8) | 0.0041 (8) | −0.0116 (9) |
| C9 | 0.0379 (9) | 0.0435 (9) | 0.0437 (9) | 0.0060 (7) | 0.0100 (7) | −0.0020 (8) |
| C10 | 0.0369 (9) | 0.0413 (9) | 0.0385 (9) | 0.0043 (7) | 0.0098 (7) | 0.0007 (7) |
| C11 | 0.0543 (11) | 0.0477 (10) | 0.0371 (9) | 0.0004 (8) | 0.0080 (8) | 0.0035 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13 | 0.0614 (11) | 0.0457 (10) | 0.0452 (10) | −0.0069 (8) | 0.0124 (9) | 0.0037 (8) |
| N1 | 0.0464 (8) | 0.0403 (8) | 0.0337 (7) | 0.0064 (6) | 0.0076 (6) | 0.0026 (6) |
| N3 | 0.0473 (9) | 0.0488 (8) | 0.0340 (7) | −0.0021 (6) | 0.0086 (7) | 0.0057 (7) |
| N14 | 0.0591 (9) | 0.0464 (8) | 0.0390 (8) | −0.0046 (7) | 0.0070 (7) | 0.0044 (7) |
| N15 | 0.0613 (10) | 0.0447 (8) | 0.0414 (8) | 0.0024 (7) | 0.0044 (7) | 0.0033 (7) |
| O1W | 0.0733 (10) | 0.0623 (9) | 0.0512 (8) | 0.0057 (8) | 0.0149 (8) | 0.0038 (6) |
| O16 | 0.1230 (16) | 0.1025 (14) | 0.0874 (12) | 0.0633 (12) | 0.0118 (11) | 0.0130 (10) |
| O17 | 0.0828 (11) | 0.0859 (11) | 0.0469 (8) | 0.0184 (8) | 0.0104 (7) | −0.0106 (7) |
| O18 | 0.1616 (18) | 0.0918 (12) | 0.0357 (8) | 0.0366 (11) | 0.0057 (10) | 0.0079 (7) |
| S12 | 0.0541 (3) | 0.0533 (3) | 0.0437 (3) | −0.0063 (2) | 0.0082 (2) | −0.0065 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C2 | 1.326 (2) | C8—C9 | 1.385 (2) |
| N1—C9 | 1.395 (2) | C8—H8 | 0.93 |
| N3—C2 | 1.327 (2) | C10—C11 | 1.359 (2) |
| N3—C4 | 1.390 (2) | C11—S12 | 1.6874 (18) |
| N14—C10 | 1.376 (2) | C11—H11 | 0.93 |
| N14—C13 | 1.296 (2) | C13—S12 | 1.7045 (19) |
| C2—C10 | 1.445 (2) | C13—H13 | 0.93 |
| C4—C9 | 1.382 (2) | N1—H1N | 0.85 (2) |
| C4—C5 | 1.383 (2) | N3—H3N | 0.82 (2) |
| C5—C6 | 1.380 (3) | N15—O18 | 1.205 (2) |
| C5—H5 | 0.93 | N15—O16 | 1.207 (2) |
| C6—C7 | 1.398 (3) | N15—O17 | 1.2516 (19) |
| C6—H6 | 0.93 | O1W—H2D | 0.85 (2) |
| C7—C8 | 1.375 (3) | O1W—H1D | 0.78 (2) |
| C7—H7 | 0.93 | | |
| | | | |
| C2—N1—C9 | 108.82 (13) | C7—C8—H8 | 121.7 |
| C2—N1—H1N | 126.9 (14) | C9—C8—H8 | 121.7 |
| C9—N1—H1N | 123.4 (13) | C4—C9—C8 | 120.69 (16) |
| C2—N3—C4 | 109.03 (14) | C4—C9—N1 | 106.34 (14) |
| C2—N3—H3N | 127.8 (15) | C8—C9—N1 | 132.97 (16) |
| C4—N3—H3N | 123.2 (15) | C11—C10—N14 | 115.50 (15) |
| N1—C2—N3 | 109.45 (15) | C11—C10—C2 | 125.47 (15) |
| N1—C2—C10 | 125.43 (14) | N14—C10—C2 | 119.03 (14) |
| N3—C2—C10 | 125.13 (15) | C10—C11—S12 | 110.26 (13) |
| C9—C4—C5 | 122.87 (17) | C10—C11—H11 | 124.9 |
| C9—C4—N3 | 106.36 (14) | S12—C11—H11 | 124.9 |
| C5—C4—N3 | 130.76 (16) | N14—C13—S12 | 116.36 (14) |
| C6—C5—C4 | 116.81 (19) | N14—C13—H13 | 121.8 |
| C6—C5—H5 | 121.6 | S12—C13—H13 | 121.8 |
| C4—C5—H5 | 121.6 | C13—N14—C10 | 108.79 (15) |
| C5—C6—C7 | 120.04 (18) | O18—N15—O16 | 120.71 (18) |
| C5—C6—H6 | 120 | O18—N15—O17 | 121.43 (17) |
| C7—C6—H6 | 120 | O16—N15—O17 | 117.84 (16) |
| C8—C7—C6 | 123.02 (19) | O18—N15—O17 | 121.43 (17) |

| | | | |
|---|---|---|---|
| C8—C7—H7 | 118.5 | O16—N15—O17 | 117.84 (16) |
| C6—C7—H7 | 118.5 | H2D—O1W—H1D | 112 (2) |
| C7—C8—C9 | 116.52 (18) | C11—S12—C13 | 89.08 (8) |
| | | | |
| C9—C4—C5—C6 | 1.6 (3) | N14—C10—C11—S12 | −0.39 (19) |
| N3—C4—C5—C6 | −179.56 (17) | C2—C10—C11—S12 | 179.16 (13) |
| C4—C5—C6—C7 | 0.2 (3) | N3—C2—N1—C9 | 0.41 (18) |
| C5—C6—C7—C8 | −2.2 (3) | C10—C2—N1—C9 | −179.28 (14) |
| C6—C7—C8—C9 | 2.3 (3) | C4—C9—N1—C2 | −0.09 (17) |
| C5—C4—C9—C8 | −1.5 (3) | C8—C9—N1—C2 | −179.72 (17) |
| N3—C4—C9—C8 | 179.44 (14) | N1—C2—N3—C4 | −0.58 (18) |
| C5—C4—C9—N1 | 178.82 (15) | C10—C2—N3—C4 | 179.11 (14) |
| N3—C4—C9—N1 | −0.25 (17) | C9—C4—N3—C2 | 0.51 (18) |
| C7—C8—C9—C4 | −0.5 (2) | C5—C4—N3—C2 | −178.47 (18) |
| C7—C8—C9—N1 | 179.10 (16) | S12—C13—N14—C10 | −0.2 (2) |
| N1—C2—C10—C11 | −179.51 (16) | C11—C10—N14—C13 | 0.4 (2) |
| N3—C2—C10—C11 | 0.8 (3) | C2—C10—N14—C13 | −179.21 (15) |
| N1—C2—C10—N14 | 0.0 (2) | C10—C11—S12—C13 | 0.22 (14) |
| N3—C2—C10—N14 | −179.62 (15) | N14—C13—S12—C11 | −0.01 (15) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H2*D*···O17 | 0.85 (2) | 2.06 (2) | 2.903 (2) | 168 (2) |
| O1*W*—H1*D*···O16$^{i}$ | 0.78 (2) | 2.24 (3) | 2.969 (2) | 156 (2) |
| N1—H1*N*···O1*W*$^{i}$ | 0.85 (2) | 1.91 (2) | 2.748 (2) | 168.5 (18) |
| N3—H3*N*···O16$^{ii}$ | 0.82 (2) | 2.58 (2) | 3.300 (2) | 147.5 (18) |
| N3—H3*N*···O17$^{ii}$ | 0.82 (2) | 2.02 (2) | 2.791 (2) | 157 (2) |

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*, *y*, *z*−1.