Di-μ-chlorido-bis[(2,2′:6,2″-terpyridine-κ^3N,N,N′)copper(II)] bis(trifluoromethanesulfonate)

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In the centrosymmetric title complex, [Cu_2Cl_2(C_15H_11N_3)_2](CF_3O_3S)_2, the Cu II metal center is fivefold coordinated by two chloride ions and three nitrogen atoms of the terpyridine ligand in a distorted square-pyramidal geometry; two trifluoromethanesulfonate ions complete the outer coordination sphere. π–π stacking interactions between the pyridyl rings in adjacent molecules contribute to the alignment of the complexes in columns along the a-axis. This structure represents the first example of a binuclear dication of formula [Cu(terpy)_2Cl_2]^{2+} with trifluoromethanesulfonate as counter-ions.

Structure description

Terpyridines are some of the most studied nitrogen-based tridentate ligands in coordination chemistry, and their metal complexes have found application in catalysis (Wei et al., 2019; Choroba et al., 2019), supramolecular chemistry (Wei et al., 2019), and medicinal chemistry (Glišić et al., 2018; Malarz et al., 2021; Li et al., 2020). Recently, copper(II) terpyridine complexes have received much attention due to their remarkable cytotoxicity and ability to interact with DNA (Karges et al., 2021); herein, we report the synthesis and structure of the title copper(II) terpyridine complex. The asymmetric unit of the title compound, depicted in Fig. 1, consists of half of a centrosymmetric dication [Cu(terpy)_2Cl_2]^{2+} and one trifluoromethanesulfonate ion completing the outer coordination sphere. The Cu–N, and Cu–Cl distances, as well as, the Cl–Cu–Cl, N–Cu–Cl and N–Cu–N angles are in good agreement with the reported values in similar copper(II) terpyridine complexes currently available in the CSD (version 5.42 with update September 2021; Rojo et al., 1987; refcode FECJEC;
Valdés-Martínez et al., 2002; refcode HULZAP; Gasser et al., 2004; refcode HULZAP01). All relevant bond lengths and angles involving the Cu atom are presented in Table 1.

In the crystal packing of the title compound, π–π stacking interactions between the N1 and N3 pyridyl ring of adjacent molecules are observed, with a centroid-to-centroid (Cg···Cg) distance of 3.658 (1) Å and an offset distance of 1.723 Å. No other supramolecular interaction is present in the crystal packing of the title compound.

Synthesis and crystallization

The title compound was obtained as product of the reaction of 2,2′:6′,2″-terpyridine (0.100 g, 0.429 mmol) with copper(II) chloride dihydrate (0.073 g, 0.429 mmol) in acetonitrile after the addition of silver trifluoromethanesulfonate (0.110 g, 0.429 mmol).

chloride dihydrate (0.073 g, 0.429 mmol) in acetonitrile after the addition of silver trifluoromethanesulfonate (0.110 g,
0.429 mmol) and filtration using a 0.45 μm PTFE syringe filter. Crystals suitable for X-ray diffraction of the title compound were obtained by vapor diffusion of diethyl ether over the resulting acetonitrile solution at 278 K.

**Refinement**

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were located in a difference map and refined in idealized positions using a riding model with atomic displacement parameters of $U_{iso}(H) = 1.2U_{eq}(C)$ and with a C—H distance of 0.95 Å.

**Acknowledgements**

We are thankful for the support of the Department of Chemistry and Biochemistry at the University of the Incarnate Word and the X-ray Diffraction Laboratory at The University of Texas at San Antonio.

**Funding information**

Funding for this research was provided by: Welch Foundation (award No. BN0032).

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full crystallographic data

IUCrData (2021). 6, x211096  [https://doi.org/10.1107/S2414314621010968]

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Crystal data

\[\text{[Cu}_2\text{Cl}_2(\text{C}_9\text{H}_11\text{N}_3)_2](\text{CF}_3\text{O}_3\text{S})_2\]

\[M_r = 962.65\]

Triclinic, \(P\overline{1}\)

\(a = 7.2767 (2) \text{ Å}\)

\(b = 9.8394 (2) \text{ Å}\)

\(c = 13.1746 (3) \text{ Å}\)

\(\alpha = 106.667 (2)^\circ\)

\(\beta = 91.226 (2)^\circ\)

\(\gamma = 105.453 (2)^\circ\)

\(V = 866.08 (4) \text{ Å}^3\)

\(Z = 1\)

\(F(000) = 482\)

\(D_x = 1.846 \text{ Mg m}^{-3}\)

Mo \(K\alpha\) radiation, \(\lambda = 0.71073 \text{ Å}\)

Cell parameters from 14071 reflections

\(\theta = 3.1–29.5^\circ\)

\(\mu = 1.59 \text{ mm}^{-1}\)

\(T = 98 \text{ K}\)

Block, clear bluish green

0.47 \times 0.17 \times 0.1 \text{ mm}

Data collection

XtaLAB AFC12 (RCD3): Kappa single diffractometer

Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source

\(\omega\) scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2019)

\(T_{\text{min}} = 0.741, T_{\text{max}} = 1.000\)

33748 measured reflections

3982 independent reflections

3889 reflections with \(I > 2\sigma(I)\)

\(R_{\text{int}} = 0.047\)

\(\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 2.3^\circ\)

\(h = -9\rightarrow9\)

\(k = -12\rightarrow12\)

\(l = -16\rightarrow17\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2\sigma(F^2)] = 0.036\)

\(wR(F^2) = 0.094\)

\(S = 1.08\)

3982 reflections

253 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

\(w = 1/[\sigma(F^2) + (0.0529P)^2 + 0.6752P]\)

where \(P = (F^2 + 2F_c^2)/3\)

\((\Delta/\sigma)_{\text{max}} = 0.002\)

\(\Delta\rho_{\text{max}} = 0.55 \text{ e Å}^{-3}\)

\(\Delta\rho_{\text{min}} = -0.41 \text{ e Å}^{-3}\)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
**Refinement.** H atoms were located in a difference map and refined in idealized positions using a riding model with atomic displacement parameters of $U_{	ext{iso}}(H) = 1.2U_{	ext{eq}}(C)$ and with a C—H distance of 0.95 Å.

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

|     | x           | y           | z           | $U_{	ext{iso}}$/U_{	ext{eq}} |
|-----|-------------|-------------|-------------|-------------------------------|
| Cu1 | 0.49265 (4) | 0.41355 (3) | 0.60172 (2) | 0.01772 (10)                 |
| Cl1 | 0.62384 (8) | 0.36614 (6) | 0.44902 (4) | 0.02026 (13)                 |
| S1  | 0.50126 (8) | 0.15121 (6) | 0.79698 (4) | 0.02142 (13)                 |
| F2  | 0.7785 (2)  | 0.02432 (18)| 0.78751 (14)| 0.0396 (4)                   |
| F1  | 0.6642 (2)  | 0.06787 (19)| 0.93864 (12)| 0.0395 (4)                   |
| F3  | 0.5041 (2)  | −0.11260 (17)| 0.80642 (16)| 0.0478 (4)                   |
| O1  | 0.6469 (2)  | 0.29199 (17)| 0.83604 (12)| 0.0239 (3)                   |
| O3  | 0.3333 (2)  | 0.1385 (2)  | 0.85354 (15)| 0.0336 (4)                   |
| O2  | 0.4661 (3)  | 0.0941 (2)  | 0.68265 (13)| 0.0360 (4)                   |
| N3  | 0.2255 (3)  | 0.27262 (19)| 0.55326 (14)| 0.0188 (4)                   |
| N2  | 0.3802 (3)  | 0.45334 (19)| 0.73563 (14)| 0.0168 (3)                   |
| N1  | 0.7290 (3)  | 0.55151 (19)| 0.70135 (14)| 0.0184 (4)                   |
| C11 | 0.1030 (3)  | 0.2851 (2)  | 0.62992 (16)| 0.0192 (4)                   |
| C5  | 0.6901 (3)  | 0.6111 (2)  | 0.80261 (16)| 0.0189 (4)                   |
| C10 | 0.1958 (3)  | 0.3840 (2)  | 0.73629 (16)| 0.0186 (4)                   |
| C6  | 0.4902 (3)  | 0.5499 (2)  | 0.82254 (16)| 0.0179 (4)                   |
| C9  | 0.1110 (3)  | 0.4087 (2)  | 0.83124 (17)| 0.0220 (4)                   |
| H9  | −0.019262   | 0.358669    | 0.833457    | 0.026*                       |
| C15 | 0.1555 (3)  | 0.1851 (2)  | 0.45439 (17)| 0.0220 (4)                   |
| H15 | 0.240897    | 0.174252    | 0.401071    | 0.026*                       |
| C14 | −0.0386 (3) | 0.1094 (2)  | 0.42706 (18)| 0.0238 (5)                   |
| H14 | −0.084305   | 0.047636    | 0.356325    | 0.029*                       |
| C12 | −0.0910 (3) | 0.2144 (2)  | 0.60811 (17)| 0.0212 (4)                   |
| H12 | −0.173957   | 0.225959    | 0.662670    | 0.025*                       |
| C13 | −0.1631 (3) | 0.1253 (2)  | 0.50390 (18)| 0.0231 (4)                   |
| H13 | −0.296333   | 0.076425    | 0.486484    | 0.028*                       |
| C7  | 0.4138 (3)  | 0.5820 (2)  | 0.91921 (16)| 0.0208 (4)                   |
| H7  | 0.489630    | 0.651756    | 0.981351    | 0.025*                       |
| C4  | 0.8284 (3)  | 0.7197 (3)  | 0.87846 (17)| 0.0225 (4)                   |
| H4  | 0.798549    | 0.759683    | 0.948670    | 0.027*                       |
| C8  | 0.2229 (3)  | 0.5089 (3)  | 0.92254 (17)| 0.0237 (5)                   |
| H8  | 0.168203    | 0.527811    | 0.988179    | 0.028*                       |
| C2  | 1.0514 (3)  | 0.7057 (3)  | 0.74756 (18)| 0.0241 (5)                   |
| H2  | 1.176548    | 0.735707    | 0.727006    | 0.029*                       |
| C16 | 0.6177 (3)  | 0.0264 (3)  | 0.83346 (19)| 0.0266 (5)                   |
| C1  | 0.9066 (3)  | 0.5979 (2)  | 0.67581 (17)| 0.0216 (4)                   |
| H1  | 0.934595    | 0.555208    | 0.605681    | 0.026*                       |
| C3  | 1.0114 (3)  | 0.7691 (3)  | 0.84983 (18)| 0.0254 (5)                   |
| H3  | 1.107711    | 0.845362    | 0.899683    | 0.030*                       |
Atomic displacement parameters (Å$^2$)

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$   | $U^{13}$   | $U^{23}$   |
|-----|------------|------------|------------|------------|------------|------------|
| Cu1 | 0.02295 (16) | 0.01815 (15) | 0.01013 (14) | 0.00641 (11) | 0.00275 (10) | 0.00076 (10) |
| Cl1 | 0.0282 (3) | 0.0213 (2) | 0.0128 (2) | 0.0121 (2) | 0.00591 (19) | 0.00269 (19) |
| S1  | 0.0221 (3) | 0.0223 (3) | 0.0156 (3) | 0.0060 (2) | −0.00080 (19) | −0.0002 (2) |
| F1  | 0.0382 (9) | 0.0427 (9) | 0.0461 (9) | 0.0246 (7) | 0.0131 (7) | 0.0132 (7) |
| F2  | 0.0508 (10) | 0.0437 (9) | 0.0241 (7) | 0.0128 (8) | −0.0061 (7) | 0.0120 (7) |
| F3  | 0.0458 (10) | 0.0206 (7) | 0.0667 (12) | 0.0001 (7) | −0.0117 (8) | 0.0074 (7) |
| O1  | 0.0284 (8) | 0.0199 (7) | 0.0201 (8) | 0.0056 (6) | 0.0030 (6) | 0.0021 (6) |
| O2  | 0.0230 (8) | 0.0371 (10) | 0.0371 (10) | 0.0075 (7) | 0.0075 (7) | 0.0065 (7) |
| N1  | 0.0262 (9) | 0.0162 (8) | 0.0132 (8) | 0.0065 (7) | 0.0020 (7) | 0.0028 (7) |
| N2  | 0.0215 (9) | 0.0152 (8) | 0.0130 (8) | 0.0063 (7) | 0.0008 (6) | 0.0021 (6) |
| N3  | 0.0239 (9) | 0.0182 (8) | 0.0133 (8) | 0.0075 (7) | 0.0024 (7) | 0.0038 (7) |
| C11 | 0.0269 (11) | 0.0159 (9) | 0.0149 (9) | 0.0073 (8) | 0.0010 (8) | 0.0037 (8) |
| C5  | 0.0248 (11) | 0.0190 (10) | 0.0141 (9) | 0.0087 (8) | 0.0032 (8) | 0.0043 (8) |
| C10 | 0.0237 (10) | 0.0167 (9) | 0.0157 (10) | 0.0073 (8) | 0.0014 (8) | 0.0039 (8) |
| C6  | 0.0234 (10) | 0.0152 (9) | 0.0144 (9) | 0.0058 (8) | 0.0014 (8) | 0.0030 (8) |
| C9  | 0.0227 (11) | 0.0225 (10) | 0.0186 (10) | 0.0053 (9) | 0.0042 (8) | 0.0039 (8) |
| C15 | 0.0332 (12) | 0.0176 (10) | 0.0144 (10) | 0.0080 (9) | 0.0016 (8) | 0.0031 (8) |
| C14 | 0.0362 (12) | 0.0149 (9) | 0.0167 (10) | 0.0056 (9) | −0.0045 (9) | 0.0011 (8) |
| C12 | 0.0247 (11) | 0.0182 (10) | 0.0205 (10) | 0.0065 (8) | 0.0017 (8) | 0.0054 (8) |
| C13 | 0.0259 (11) | 0.0158 (10) | 0.0246 (11) | 0.0040 (8) | −0.0045 (9) | 0.0039 (8) |
| C7  | 0.0256 (11) | 0.0210 (10) | 0.0122 (9) | 0.0061 (9) | 0.0010 (8) | 0.0000 (8) |
| C4  | 0.0261 (11) | 0.0241 (11) | 0.0157 (10) | 0.0088 (9) | 0.0031 (8) | 0.0020 (8) |
| C8  | 0.0282 (12) | 0.0277 (11) | 0.0134 (10) | 0.0087 (9) | 0.0055 (8) | 0.0025 (8) |
| C2  | 0.0215 (11) | 0.0285 (11) | 0.0233 (11) | 0.0074 (9) | 0.0034 (8) | 0.0093 (9) |
| C16 | 0.0308 (12) | 0.0197 (10) | 0.0240 (11) | 0.0049 (9) | −0.0022 (9) | 0.0010 (9) |
| C1  | 0.0266 (11) | 0.0250 (11) | 0.0166 (10) | 0.0114 (9) | 0.0055 (8) | 0.0075 (8) |
| C3  | 0.0256 (11) | 0.0275 (11) | 0.0198 (11) | 0.0063 (9) | −0.0014 (9) | 0.0036 (9) |

Geometric parameters (Å, °)

| Cu1—Cl1 | 2.2265 (5) | C10—C9 | 1.394 (3) |
| Cu1—Cl1 | 2.7660 (6) | C6—C7 | 1.387 (3) |
| Cu1—N3 | 2.0278 (19) | C9—H9 | 0.9500 |
| Cu1—N2 | 1.9420 (17) | C9—C8 | 1.390 (3) |
| Cu1—N1 | 2.0397 (18) | C15—H15 | 0.9500 |
| S1—O1 | 1.4466 (17) | C15—C14 | 1.394 (3) |
| S1—N3 | 1.4409 (18) | C14—H14 | 0.9500 |
| S1—O2 | 1.4392 (17) | C14—C13 | 1.376 (3) |
| S1—C6 | 1.826 (2) | C12—H12 | 0.9500 |
| F2—C16 | 1.331 (3) | C12—C13 | 1.401 (3) |
| F1—C16 | 1.335 (3) | C13—H13 | 0.9500 |
| F3—C16 | 1.337 (3) | C7—H7 | 0.9500 |
| N3—C11 | 1.362 (3) | C7—C8 | 1.392 (3) |
| N3—C15 | 1.339 (3) | C4—H4 | 0.9500 |
| Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|--------------|--------------|--------------|
| N2—C10       | 1.335 (3)    | C4—C3        | 1.391 (3)    |
| N2—C6        | 1.336 (3)    | C8—H8        | 0.9500       |
| N1—C5        | 1.364 (3)    | C2—H2        | 0.9500       |
| N1—C1        | 1.336 (3)    | C2—C1        | 1.384 (3)    |
| C11—C10      | 1.481 (3)    | C2—C3        | 1.386 (3)    |
| C11—C12      | 1.380 (3)    | C1—H1        | 0.9500       |
| C5—C6        | 1.479 (3)    | C3—H3        | 0.9500       |
| C5—C4        | 1.388 (3)    |              |              |
| Cl1—Cu1—Cl1' | 89.944 (18)  | C8—C9—C10    | 117.9 (2)    |
| N3—Cu1—Cl1' | 90.30 (5)    | C8—C9—H9     | 121.0        |
| N3—Cu1—Cl1   | 99.82 (5)    | N3—C15—H15   | 118.9        |
| N3—Cu1—N1    | 159.58 (7)   | N3—C15—C14   | 122.2 (2)    |
| N2—Cu1—Cl1' | 90.83 (5)    | C14—C15—H15  | 118.9        |
| N2—Cu1—Cl1   | 179.20 (5)   | C15—C14—H14  | 120.4        |
| N2—Cu1—N3    | 80.39 (7)    | C13—C14—C15  | 119.1 (2)    |
| N2—Cu1—N1    | 80.11 (7)    | C13—C14—H14  | 120.4        |
| N1—Cu1—Cl1   | 99.60 (5)    | C11—C12—H12  | 120.7        |
| N1—Cu1—Cl1' | 95.97 (5)    | C11—C12—C13  | 118.7 (2)    |
| Cu1—Cl1—Cu1' | 90.056 (18)  | C13—C12—H12  | 120.7        |
| O1—S1—C16    | 102.05 (10)  | C14—C13—C12  | 119.2 (2)    |
| O3—S1—O1     | 114.97 (10)  | C14—C13—H13  | 120.4        |
| O3—S1—C16    | 103.57 (11)  | C12—C13—H13  | 120.4        |
| O2—S1—O1     | 114.19 (11)  | C6—C7—H7     | 121.0        |
| O2—S1—O3     | 115.73 (12)  | C6—C7—C8     | 118.1 (2)    |
| O2—S1—C16    | 103.90 (11)  | C8—C7—H7     | 121.0        |
| C11—N3—Cu1   | 113.61 (14)  | C5—C4—H4     | 120.6        |
| C15—N3—Cu1   | 127.30 (15)  | C5—C4—C3     | 118.8 (2)    |
| C15—N3—C11   | 118.61 (19)  | C3—C4—H4     | 120.6        |
| C10—N2—Cu1   | 118.38 (14)  | C9—C8—C7     | 121.0 (2)    |
| C10—N2—C6    | 123.04 (18)  | C9—C8—H8     | 119.5        |
| C6—N2—Cu1    | 118.58 (14)  | C7—C8—H8     | 119.5        |
| C5—N1—Cu1    | 113.57 (14)  | C1—C2—H2     | 120.5        |
| C1—N1—Cu1    | 127.51 (15)  | C1—C2—C3     | 119.1 (2)    |
| C1—N1—C5     | 118.60 (19)  | C3—C2—H2     | 120.5        |
| N3—C11—C10   | 114.06 (19)  | F2—C16—S1    | 111.78 (16)  |
| N3—C11—C12   | 122.2 (2)    | F2—C16—F1    | 107.3 (2)    |
| C12—C11—C10  | 123.8 (2)    | F2—C16—F3    | 107.8 (2)    |
| N1—C5—C6     | 114.01 (18)  | F1—C16—S1    | 110.99 (16)  |
| N1—C5—C4     | 121.9 (2)    | F1—C16—F3    | 106.5 (2)    |
| C4—C5—C6     | 124.13 (19)  | F3—C16—S1    | 112.25 (17)  |
| N2—C10—C11   | 113.09 (18)  | N1—C1—C2     | 122.5 (2)    |
| N2—C10—C9    | 119.91 (19)  | N1—C1—H1     | 118.7        |
| C9—C10—C11   | 127.0 (2)    | C2—C1—H1     | 118.7        |
| N2—C6—C5     | 113.29 (18)  | C4—C3—H3     | 120.5        |
| N2—C6—C7     | 120.03 (19)  | C2—C3—C4     | 119.1 (2)    |
| C7—C6—C5     | 126.68 (19)  | C2—C3—H3     | 120.5        |
| C10—C9—H9    | 121.0        |              |              |
Cu1—N3—C11—C10  -7.7 (2)  N1—C5—C4—C3  0.2 (3)
Cu1—N3—C11—C12  170.55 (16)  C11—N3—C15—C14  1.5 (3)
Cu1—N3—C15—C14  -170.07 (15)  C11—C10—C9—C8  -178.6 (2)
Cu1—N2—C10—C11  -0.7 (2)  C11—C12—C13—C14  0.8 (3)
Cu1—N2—C10—C9   179.33 (15)  C5—N1—C1—C2   -1.1 (3)
Cu1—N2—C6—C5    -1.4 (2)  C5—C6—C7—C8   -177.9 (2)
Cu1—N2—C6—C7    179.33 (15)  C5—C4—C3—C2   -1.7 (3)
Cu1—N1—C5—C6    7.0 (2)  C10—N2—C6—C5   179.27 (18)
Cu1—N1—C5—C4  -172.78 (16)  C10—N2—C6—C7   0.0 (3)
Cu1—N1—C1—C2  171.97 (16)  C10—C11—C12—C13  178.98 (19)
O1—S1—C16—F2  -60.24 (18)  C10—C9—C8—C7   -0.1 (3)
O1—S1—C16—F1  59.49 (19)  C6—N2—C10—C11  178.63 (18)
O1—S1—C16—F3  178.50 (17)  C6—N2—C10—C9   -1.4 (3)
O3—S1—C16—F2  -179.95 (16)  C6—C5—C4—C3   -179.6 (2)
O3—S1—C16—F1  -60.22 (19)  C6—C7—C8—C9   -1.1 (3)
O3—S1—C16—F3  58.8 (2)  C15—N3—C11—C10  179.69 (18)
O2—S1—C16—F2  58.73 (19)  C15—N3—C11—C12  -2.1 (3)
O2—S1—C16—F1  178.47 (17)  C15—C14—C13—C12  -1.5 (3)
O2—S1—C16—F3  -62.5 (2)  C12—C11—C10—N2   -172.60 (19)
N3—C11—C10—N2  5.6 (3)  C12—C11—C10—C9   7.4 (3)
N3—C11—C10—C9  -174.4 (2)  C4—C5—C6—N2   175.9 (2)
N3—C11—C12—C13  1.0 (3)  C4—C5—C6—C7  -4.9 (3)
N3—C15—C14—C13  0.3 (3)  C1—N1—C5—C6   -178.99 (18)
N2—C10—C9—C8  1.4 (3)  C1—N1—C5—C4   1.3 (3)
N2—C6—C7—C8  1.2 (3)  C1—C2—C3—C4  1.9 (3)
N1—C5—C6—N2  -3.8 (3)  C3—C2—C1—N1  -0.4 (3)
N1—C5—C6—C7  175.3 (2)

Symmetry code: (i) −x+1, −y+1, −z+1.