

Bis[bis(3,5-diamino-1*H*-1,2,4-triazol-4-ium)copper(I)] tris(hexafluorosilicate)

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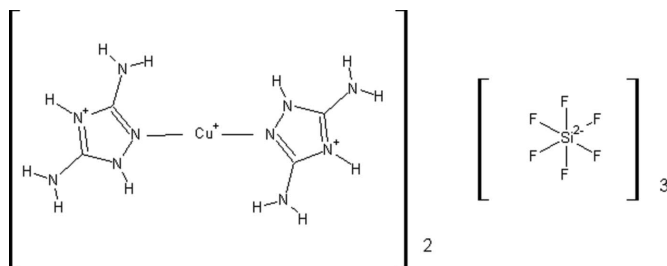
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{N}-\text{C}) = 0.004$ Å; R factor = 0.053; wR factor = 0.155; data-to-parameter ratio = 16.8.

In the title compound, $[\text{Cu}(\text{C}_2\text{H}_6\text{N}_5)_2]_2(\text{SiF}_6)_3$, the asymmetric unit is composed of one $[\text{Cu}(\text{HL})_2]^{3+}$ cation (where L is 3,5-diamino-1,2,4-triazole) and one and a half SiF_6^{2-} anions. The rather large positively charged guanazole ligand moiety promotes the low metal coordination number of 2 for the Cu^{I} atom. The compound was obtained using the electrochemical alternating-current technique starting from an ethanol-methanol solution of $\text{CuSiF}_6 \cdot 4\text{H}_2\text{O}$ and guanazole. In the crystal, $\text{N}-\text{H} \cdots \text{F}$ hydrogen bonds play an important role in the formation of a three-dimensional network. As a result of these hydrogen bonds, there are also $\pi-\pi$ interactions [centroid-centroid distance = $3.3024(14)$ Å] involving one of the triazole groups in molecules related by an inversion center, and short $\text{Cu} \cdots \text{N}$ interactions [$2.909(3)$ Å] involving an $-\text{NH}_2$ group, leading to the formation of a dimer-like arrangement.

Related literature

For 1,2,4-triazole and its functionalized derivatives, see: Potts (1984). For complexes of the same ligand and copper(I) complexes of similar voluminous ligands, see: Aznar *et al.* (2006); Fabretti (1992); Goreshnik *et al.* (2004).



Experimental

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_6\text{N}_5)_2]_2(\text{SiF}_6)_3$
 $M_r = 953.84$
 Triclinic, $P\bar{1}$
 $a = 7.482(2)$ Å
 $b = 8.366(1)$ Å
 $c = 12.131(3)$ Å
 $\alpha = 87.98(2)^\circ$
 $\beta = 89.11(2)^\circ$

$\gamma = 67.89(2)^\circ$
 $V = 703.1(3)$ Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 1.81$ mm⁻¹
 $T = 293$ K
 $0.24 \times 0.20 \times 0.04$ mm

Data collection

Siemens AED2 diffractometer
 Absorption correction: numerical
 (de Meulanaer & Tompa, 1965)
 $T_{\text{min}} = 0.649$, $T_{\text{max}} = 0.935$
 4089 measured reflections

4089 independent reflections
 3367 reflections with $I > 2\sigma(I)$
 3 standard reflections every 60 min
 intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.155$
 $S = 1.06$
 4089 reflections
 244 parameters
 4 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.01$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|---|--------------|---------------------|--------------|-----------------------|
| $\text{N}2-\text{H}2 \cdots \text{F}2^{\text{i}}$ | 0.86 (2) | 1.86 (2) | 2.694 (3) | 166 (4) |
| $\text{N}3-\text{H}3 \cdots \text{F}8$ | 0.88 (2) | 2.02 (3) | 2.798 (3) | 146 (4) |
| $\text{N}4-\text{H}4\text{B} \cdots \text{F}1^{\text{ii}}$ | 0.86 | 1.95 | 2.742 (4) | 153 |
| $\text{N}4-\text{H}4\text{A} \cdots \text{F}9^{\text{ii}}$ | 0.86 | 1.95 | 2.801 (3) | 171 |
| $\text{N}5-\text{H}5\text{A} \cdots \text{F}6^{\text{iii}}$ | 0.86 | 1.95 | 2.803 (3) | 174 |
| $\text{N}5-\text{H}5\text{B} \cdots \text{F}9^{\text{iv}}$ | 0.86 | 2.07 | 2.898 (3) | 162 |
| $\text{N}7-\text{H}7 \cdots \text{F}4^{\text{i}}$ | 0.86 (2) | 1.85 (2) | 2.686 (3) | 162 (4) |
| $\text{N}8-\text{H}8 \cdots \text{F}7^{\text{v}}$ | 0.86 (2) | 2.04 (3) | 2.812 (3) | 148 (4) |
| $\text{N}8-\text{H}8 \cdots \text{F}3^{\text{v}}$ | 0.86 (2) | 2.22 (3) | 2.813 (3) | 126 (3) |
| $\text{N}9-\text{H}9\text{B} \cdots \text{F}8^{\text{vi}}$ | 0.86 | 2.05 | 2.892 (3) | 166 |
| $\text{N}9-\text{H}9\text{A} \cdots \text{F}5^{\text{vii}}$ | 0.86 | 2.02 | 2.841 (4) | 159 |
| $\text{N}10-\text{H}10\text{B} \cdots \text{F}5^{\text{v}}$ | 0.86 | 2.22 | 2.909 (3) | 137 |
| $\text{N}10-\text{H}10\text{A} \cdots \text{F}6^{\text{iii}}$ | 0.86 | 2.02 | 2.845 (3) | 160 |

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+1, -z$; (iii) $x, y-1, z$; (iv) $-x+2, -y, -z$; (v) $-x+1, -y, -z+1$; (vi) $x-1, y, z+1$; (vii) $-x, -y+1, -z+1$.

Data collection: *STADIA* (Stoe & Cie, 1998); cell refinement: *STADIA*; data reduction: *X-RED* (Stoe & Cie, 1998); program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Crystal Impact, 2010), *ORTEP-III* (Burnett & Johnson, 1996) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2214).

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supporting information

Acta Cryst. (2010). E66, m1453–m1454 [https://doi.org/10.1107/S160053681004225X]

Bis[bis(3,5-diamino-1*H*-1,2,4-triazol-4-ium)copper(I)] tris(hexafluorosilicate)**Marian Mys'kiv and Evgeny Goreshnik****S1. Comment**

1,2,4-triazole and its functionalized derivatives, particularly 3,5-diamino-1,2,4-triazole (*L*), have attracted great interest and are actively studied as ligands in the synthesis of coordination compounds, biologically active compounds with a wide range efficiency, and as components of high-energy compositions [Potts, 1984]. On the other hand only a few X-ray crystal structures of complexes of this triazole have been reported (Aznar *et al.*, 2006). The formation of low soluble polynuclear metal derivatives is one of the hindrances for structural studies of such compounds. It may be expected that the protonated form of the ligand (LH) will possess lower affinity to metal centers. Herein, we report on the synthesis and crystal structure of the title copper(I) hexafluorosilicate complex of LH.

Beside the positively charged state, the LH moiety demonstrates ability of metal coordination. In the structure of $[\text{Cu}(\text{LH})_2]_2(\text{SiF}_6)_3$ each metal atom is bound to two nitrogen atoms from two LH moieties (Fig. 1). A similar linear copper(I) surrounding comprising of two nitrogen atoms from two voluminous ligand molecules was observed, for example, in the structure of bis(2-methylbenzimidazole)copper(I) dichlorocuprate(I) (Goreshnik *et al.*, 2004). Because of the low copper(I) ion coordination number both Cu–N distances appear to be rather short, 1.8747 (18) and 1.8749 (17) Å. Despite the cationic status of the ligand moiety the Cu–N bond length is practically the same [1.874 (2) Å] as in the above mentioned bis(2-methylbenzimidazole)copper(I) cation.

In the crystal each NH and NH₂ hydrogen atom participates in the formation of strong N—H...F hydrogen bonds (Table 1). The closest NH₂ group to the coordinated copper ion $[\text{Cu}1 \cdots \text{N}10^i = 2.9092 (29) \text{ \AA}$, symmetry code (i) = $-x + 1, -y, -z + 1$], forms noticeably shorter hydrogen bonds than all the others. Each of the two crystallographically independent SiF₆²⁻ anions is bound to six LH units (Fig. 2). The $[\text{Cu}(\text{LH})]^{3+}$ and SiF₆²⁻ units are interconnected by N—H...F bonds to form a three dimensional network (Fig. 3). In the crystal there are also π – π interactions involving triazole rings (N1—N3, C3, C4 = Cg2) related by an inversion center, with a centroid-to-centroid distance of 3.3024 (14) Å for Cg2...Cg2ⁱⁱ [symmetry code (ii) = $-x, -y, 1 - z$].

As was already mentioned, the guanazolium moiety in this structure acts as a ligand despite its cationic status. Such behaviour was observed previously in the structure of platinum(II) dibromo bis(3,5-diamino-1(2)-triazolium) dibromide (Fabretti, 1992). It emphasizes the high affinity of this triazole derivative towards metal ions. The relatively large size of the LH units and their positive charge lead to the low coordination number of the copper ion.

S2. Experimental

The title compound was prepared using electrochemical synthesis. An ethanol solution of (LH)₂SiF₆ (where *L* = 3,5-diamino-1,2,4-triazole) was added to a solution of Cu₂SiF₆·4H₂O (prepared by dissolving [(CuOH)₂CO₃] in H₂SiF₆) in CH₃OH. This solution was then placed in a small test-tube and copper-wire electrodes were inserted. By usage of the alternating-current electrochemical technique at 0.5 V of tension during some days colourless crystals of the title compound appeared on the electrodes.

S3. Refinement

The N-bound H-atoms could all be located in difference Fourier maps. In the final cycles of least-squares refinement they were refined with distance restraints of 0.86 (2) Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

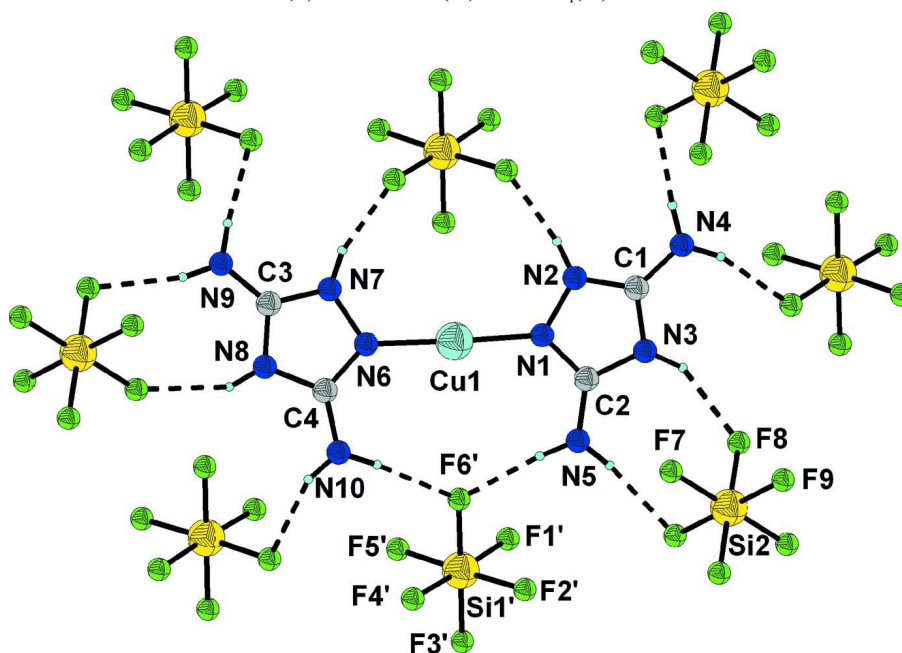


Figure 1

Copper surrounding of the title cation with displacement ellipsoids drawn at the 50% probability level [Symmetry operation: (') = x, y-1, z].

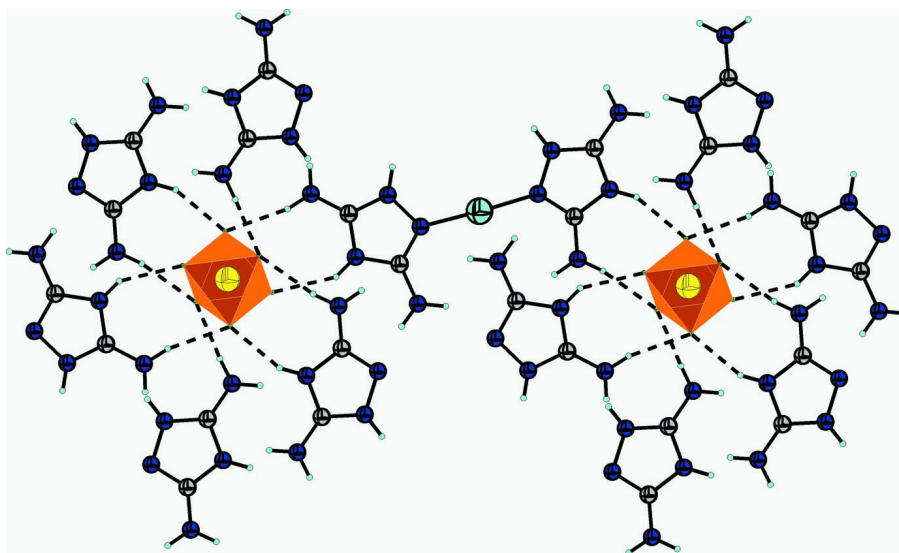


Figure 2

The environment of the SiF₆²⁻ dianions in the title compound.

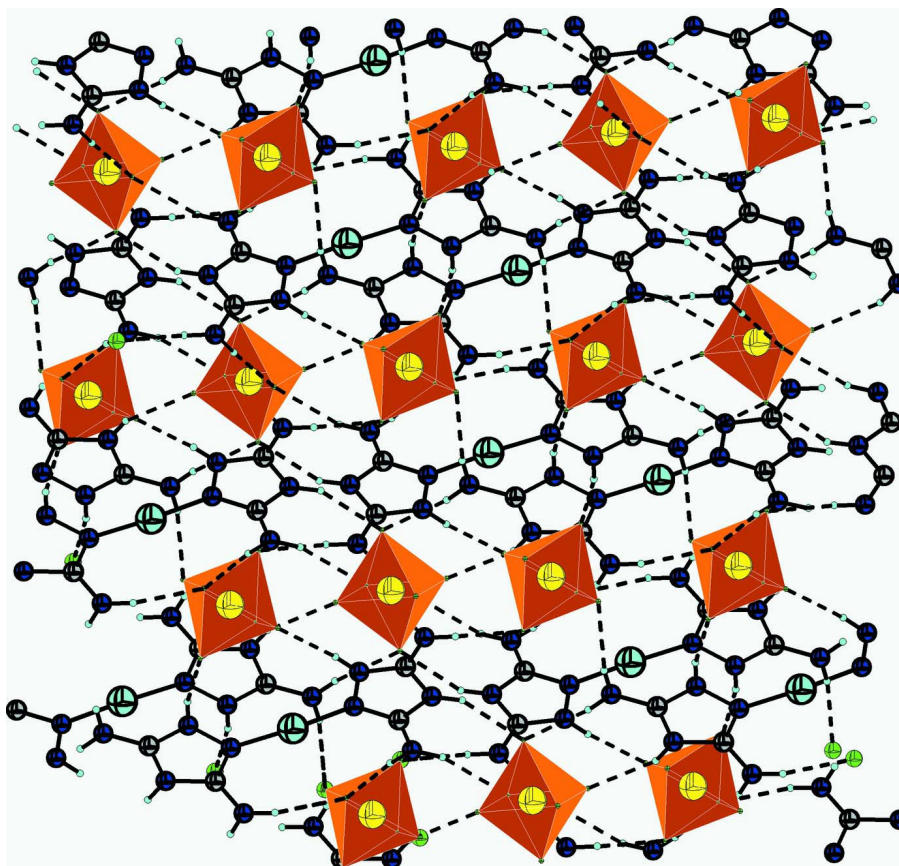


Figure 3

A view along the b-axis of the crystal packing of the title compound.

Bis[bis(3,5-diamino-1H-1,2,4-triazol-4-ium)copper(I)] tris(hexafluorosilicate)

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_6\text{N}_5)_2]_2(\text{SiF}_6)_3$

$M_r = 953.84$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.482$ (2) Å

$b = 8.366$ (1) Å

$c = 12.131$ (3) Å

$\alpha = 87.98$ (2)°

$\beta = 89.11$ (2)°

$\gamma = 67.89$ (2)°

$V = 703.1$ (3) Å³

$Z = 1$

$F(000) = 474$

$D_x = 2.253$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 25 reflections

$\theta = 35\text{--}45^\circ$

$\mu = 1.81$ mm⁻¹

$T = 293$ K

Plate, colourless

$0.24 \times 0.20 \times 0.04$ mm

Data collection

Siemens AED2

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\theta/2\omega$ scans

Absorption correction: numerical

(de Meulanaer & Tompa, 1965)

$T_{\min} = 0.649$, $T_{\max} = 0.935$

4089 measured reflections

4089 independent reflections

3367 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.000$

$\theta_{\max} = 30.0^\circ$, $\theta_{\min} = 1.7^\circ$

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 11$
 $l = 0 \rightarrow 17$

3 standard reflections every 60 min
 intensity decay: 2%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.155$
 $S = 1.06$
 4089 reflections
 244 parameters
 4 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
 $w = 1/[\sigma^2(F_o^2) + (0.1004P)^2 + 0.624P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.01 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|-------------|--------------|----------------------------------|
| Cu1 | 0.23338 (6) | 0.16548 (5) | 0.35785 (3) | 0.03274 (14) |
| N1 | 0.2950 (4) | 0.2228 (3) | 0.2154 (2) | 0.0266 (5) |
| N2 | 0.1956 (4) | 0.3827 (3) | 0.1626 (2) | 0.0286 (5) |
| H2 | 0.084 (4) | 0.453 (5) | 0.182 (3) | 0.034* |
| N3 | 0.4365 (3) | 0.2455 (3) | 0.0583 (2) | 0.0248 (5) |
| H3 | 0.512 (5) | 0.226 (5) | 0.000 (2) | 0.030* |
| N4 | 0.2278 (5) | 0.5262 (4) | -0.0040 (2) | 0.0389 (7) |
| H4A | 0.1265 | 0.6165 | 0.0081 | 0.047* |
| H4B | 0.2942 | 0.5211 | -0.0632 | 0.047* |
| N5 | 0.5685 (4) | -0.0176 (3) | 0.1625 (2) | 0.0322 (6) |
| H5A | 0.5625 | -0.0792 | 0.2197 | 0.039* |
| H5B | 0.6580 | -0.0594 | 0.1143 | 0.039* |
| N6 | 0.1586 (3) | 0.1111 (3) | 0.49796 (19) | 0.0236 (4) |
| N7 | -0.0093 (4) | 0.2215 (3) | 0.54935 (19) | 0.0245 (5) |
| H7 | -0.091 (5) | 0.318 (3) | 0.524 (3) | 0.029* |
| N8 | 0.1222 (3) | 0.0061 (3) | 0.66222 (19) | 0.0238 (4) |
| H8 | 0.132 (6) | -0.065 (4) | 0.717 (2) | 0.029* |
| N9 | -0.1716 (4) | 0.2238 (4) | 0.7183 (2) | 0.0342 (6) |
| H9A | -0.2647 | 0.3194 | 0.7016 | 0.041* |
| H9B | -0.1717 | 0.1722 | 0.7809 | 0.041* |
| N10 | 0.4006 (4) | -0.1545 (3) | 0.5565 (2) | 0.0296 (5) |
| H10A | 0.4684 | -0.1618 | 0.4976 | 0.036* |

| | | | | |
|------|--------------|-------------|---------------|--------------|
| H10B | 0.4393 | -0.2340 | 0.6074 | 0.036* |
| C1 | 0.2813 (4) | 0.3948 (4) | 0.0686 (2) | 0.0257 (5) |
| C2 | 0.4398 (4) | 0.1416 (4) | 0.1488 (2) | 0.0226 (5) |
| C3 | -0.0290 (4) | 0.1567 (4) | 0.6484 (2) | 0.0230 (5) |
| C4 | 0.2343 (4) | -0.0189 (3) | 0.5689 (2) | 0.0215 (5) |
| Si1 | 0.68995 (11) | 0.55369 (9) | 0.31802 (7) | 0.02457 (18) |
| F1 | 0.5751 (3) | 0.5922 (3) | 0.19565 (17) | 0.0403 (5) |
| F2 | 0.8718 (3) | 0.5985 (3) | 0.25878 (19) | 0.0408 (5) |
| F3 | 0.8049 (4) | 0.3448 (3) | 0.2924 (2) | 0.0525 (6) |
| F4 | 0.7987 (3) | 0.5232 (3) | 0.44239 (19) | 0.0426 (5) |
| F5 | 0.5036 (3) | 0.5137 (3) | 0.37463 (18) | 0.0370 (4) |
| F6 | 0.5785 (3) | 0.7657 (2) | 0.34582 (15) | 0.0305 (4) |
| Si2 | 1.0000 | 0.0000 | 0.0000 | 0.0211 (2) |
| F7 | 0.9165 (3) | 0.0973 (3) | 0.11859 (16) | 0.0347 (4) |
| F8 | 0.7827 (3) | 0.1080 (3) | -0.05936 (16) | 0.0344 (4) |
| F9 | 1.0741 (3) | 0.1610 (2) | -0.03969 (18) | 0.0344 (4) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|---------------|--------------|--------------|
| Cu1 | 0.0426 (2) | 0.0340 (2) | 0.0220 (2) | -0.01538 (17) | 0.01182 (15) | 0.00019 (14) |
| N1 | 0.0254 (11) | 0.0263 (11) | 0.0219 (11) | -0.0033 (9) | 0.0087 (8) | 0.0016 (8) |
| N2 | 0.0266 (11) | 0.0262 (11) | 0.0235 (11) | 0.0004 (9) | 0.0108 (9) | -0.0012 (9) |
| N3 | 0.0242 (10) | 0.0222 (10) | 0.0244 (11) | -0.0048 (9) | 0.0127 (8) | -0.0032 (8) |
| N4 | 0.0456 (16) | 0.0234 (12) | 0.0305 (13) | 0.0056 (11) | 0.0124 (11) | 0.0047 (10) |
| N5 | 0.0250 (11) | 0.0271 (12) | 0.0372 (14) | -0.0022 (9) | 0.0096 (10) | 0.0048 (10) |
| N6 | 0.0254 (10) | 0.0238 (10) | 0.0204 (10) | -0.0081 (8) | 0.0065 (8) | -0.0014 (8) |
| N7 | 0.0259 (11) | 0.0228 (10) | 0.0208 (10) | -0.0049 (9) | 0.0040 (8) | 0.0014 (8) |
| N8 | 0.0225 (10) | 0.0276 (11) | 0.0200 (10) | -0.0084 (9) | 0.0051 (8) | 0.0010 (8) |
| N9 | 0.0238 (11) | 0.0422 (15) | 0.0272 (12) | -0.0021 (10) | 0.0094 (9) | 0.0018 (10) |
| N10 | 0.0252 (11) | 0.0258 (12) | 0.0319 (13) | -0.0033 (9) | 0.0076 (9) | -0.0002 (9) |
| C1 | 0.0280 (13) | 0.0222 (12) | 0.0223 (12) | -0.0041 (10) | 0.0100 (10) | -0.0043 (9) |
| C2 | 0.0194 (11) | 0.0240 (12) | 0.0219 (12) | -0.0057 (9) | 0.0071 (9) | -0.0012 (9) |
| C3 | 0.0209 (11) | 0.0275 (13) | 0.0204 (11) | -0.0090 (10) | 0.0036 (9) | -0.0012 (9) |
| C4 | 0.0230 (11) | 0.0223 (11) | 0.0204 (11) | -0.0102 (9) | 0.0042 (9) | -0.0006 (9) |
| Si1 | 0.0230 (3) | 0.0170 (3) | 0.0284 (4) | -0.0017 (3) | 0.0092 (3) | -0.0018 (3) |
| F1 | 0.0443 (11) | 0.0473 (12) | 0.0260 (9) | -0.0130 (9) | 0.0055 (8) | -0.0072 (8) |
| F2 | 0.0294 (9) | 0.0356 (10) | 0.0544 (13) | -0.0091 (8) | 0.0225 (9) | -0.0072 (9) |
| F3 | 0.0511 (13) | 0.0212 (9) | 0.0772 (17) | -0.0041 (9) | 0.0209 (12) | -0.0134 (10) |
| F4 | 0.0439 (11) | 0.0338 (10) | 0.0439 (12) | -0.0083 (9) | -0.0108 (9) | 0.0122 (9) |
| F5 | 0.0336 (9) | 0.0348 (10) | 0.0425 (11) | -0.0134 (8) | 0.0122 (8) | 0.0030 (8) |
| F6 | 0.0348 (9) | 0.0183 (7) | 0.0297 (9) | -0.0005 (6) | 0.0104 (7) | -0.0020 (6) |
| Si2 | 0.0195 (4) | 0.0196 (4) | 0.0209 (5) | -0.0037 (3) | 0.0087 (3) | -0.0007 (3) |
| F7 | 0.0376 (10) | 0.0352 (10) | 0.0269 (9) | -0.0087 (8) | 0.0158 (7) | -0.0087 (7) |
| F8 | 0.0236 (8) | 0.0379 (10) | 0.0326 (9) | -0.0019 (7) | 0.0047 (7) | 0.0052 (8) |
| F9 | 0.0327 (9) | 0.0246 (8) | 0.0454 (11) | -0.0108 (7) | 0.0164 (8) | -0.0009 (7) |

Geometric parameters (Å, °)

| | | | |
|------------|-------------|--------------------------------------|-------------|
| Cu1—N1 | 1.874 (2) | N8—C4 | 1.372 (3) |
| Cu1—N6 | 1.875 (2) | N8—H8 | 0.864 (19) |
| N1—C2 | 1.321 (3) | N9—C3 | 1.315 (3) |
| N1—N2 | 1.399 (4) | N9—H9A | 0.8600 |
| N2—C1 | 1.320 (3) | N9—H9B | 0.8600 |
| N2—H2 | 0.856 (19) | N10—C4 | 1.342 (4) |
| N3—C1 | 1.356 (3) | N10—H10A | 0.8600 |
| N3—C2 | 1.371 (4) | N10—H10B | 0.8600 |
| N3—H3 | 0.877 (19) | Si1—F3 | 1.670 (2) |
| N4—C1 | 1.324 (4) | Si1—F5 | 1.683 (2) |
| N4—H4A | 0.8600 | Si1—F1 | 1.686 (2) |
| N4—H4B | 0.8600 | Si1—F2 | 1.686 (2) |
| N5—C2 | 1.324 (4) | Si1—F4 | 1.691 (2) |
| N5—H5A | 0.8600 | Si1—F6 | 1.6959 (19) |
| N5—H5B | 0.8600 | Si2—F7 ⁱ | 1.6716 (18) |
| N6—C4 | 1.316 (4) | Si2—F7 | 1.6716 (18) |
| N6—N7 | 1.401 (3) | Si2—F9 ⁱ | 1.6912 (18) |
| N7—C3 | 1.329 (4) | Si2—F9 | 1.6912 (18) |
| N7—H7 | 0.863 (19) | Si2—F8 | 1.6920 (19) |
| N8—C3 | 1.347 (4) | Si2—F8 ⁱ | 1.6920 (19) |
| | | | |
| N1—Cu1—N6 | 177.04 (11) | N9—C3—N7 | 126.7 (3) |
| C2—N1—N2 | 105.2 (2) | N9—C3—N8 | 126.3 (3) |
| C2—N1—Cu1 | 131.5 (2) | N7—C3—N8 | 106.9 (2) |
| N2—N1—Cu1 | 122.95 (18) | N6—C4—N10 | 126.3 (2) |
| C1—N2—N1 | 110.1 (2) | N6—C4—N8 | 110.1 (2) |
| C1—N2—H2 | 125 (3) | N10—C4—N8 | 123.5 (3) |
| N1—N2—H2 | 124 (3) | F3—Si1—F5 | 90.85 (12) |
| C1—N3—C2 | 107.6 (2) | F3—Si1—F1 | 91.99 (14) |
| C1—N3—H3 | 122 (3) | F5—Si1—F1 | 88.81 (12) |
| C2—N3—H3 | 131 (3) | F3—Si1—F2 | 90.24 (12) |
| C1—N4—H4A | 120.0 | F5—Si1—F2 | 178.23 (12) |
| C1—N4—H4B | 120.0 | F1—Si1—F2 | 89.76 (12) |
| H4A—N4—H4B | 120.0 | F3—Si1—F4 | 90.31 (14) |
| C2—N5—H5A | 120.0 | F5—Si1—F4 | 90.60 (12) |
| C2—N5—H5B | 120.0 | F1—Si1—F4 | 177.64 (12) |
| H5A—N5—H5B | 120.0 | F2—Si1—F4 | 90.79 (13) |
| C4—N6—N7 | 104.9 (2) | F3—Si1—F6 | 178.49 (13) |
| C4—N6—Cu1 | 133.6 (2) | F5—Si1—F6 | 90.04 (10) |
| N7—N6—Cu1 | 121.44 (18) | F1—Si1—F6 | 89.24 (11) |
| C3—N7—N6 | 110.1 (2) | F2—Si1—F6 | 88.90 (11) |
| C3—N7—H7 | 122 (3) | F4—Si1—F6 | 88.47 (11) |
| N6—N7—H7 | 128 (3) | F7 ⁱ —Si2—F7 | 180.00 (15) |
| C3—N8—C4 | 107.9 (2) | F7 ⁱ —Si2—F9 ⁱ | 90.37 (10) |
| C3—N8—H8 | 123 (3) | F7—Si2—F9 ⁱ | 89.63 (10) |
| C4—N8—H8 | 129 (3) | F7 ⁱ —Si2—F9 | 89.63 (10) |

| | | | |
|---------------|--------------|--------------------------------------|-------------|
| C3—N9—H9A | 120.0 | F7—Si2—F9 | 90.37 (10) |
| C3—N9—H9B | 120.0 | F9 ⁱ —Si2—F9 | 180.00 (16) |
| H9A—N9—H9B | 120.0 | F7 ⁱ —Si2—F8 | 90.01 (10) |
| C4—N10—H10A | 120.0 | F7—Si2—F8 | 89.99 (10) |
| C4—N10—H10B | 120.0 | F9 ⁱ —Si2—F8 | 89.66 (10) |
| H10A—N10—H10B | 120.0 | F9—Si2—F8 | 90.34 (10) |
| N2—C1—N4 | 127.3 (3) | F7 ⁱ —Si2—F8 ⁱ | 89.99 (10) |
| N2—C1—N3 | 107.2 (3) | F7—Si2—F8 ⁱ | 90.01 (10) |
| N4—C1—N3 | 125.4 (3) | F9 ⁱ —Si2—F8 ⁱ | 90.34 (10) |
| N1—C2—N5 | 126.8 (3) | F9—Si2—F8 ⁱ | 89.66 (10) |
| N1—C2—N3 | 109.8 (2) | F8—Si2—F8 ⁱ | 180.00 (12) |
| N5—C2—N3 | 123.3 (2) | | |
| | | | |
| N6—Cu1—N1—C2 | -133 (2) | N2—N1—C2—N3 | 1.2 (3) |
| N6—Cu1—N1—N2 | 54 (2) | Cu1—N1—C2—N3 | -172.2 (2) |
| C2—N1—N2—C1 | -0.6 (3) | C1—N3—C2—N1 | -1.3 (3) |
| Cu1—N1—N2—C1 | 173.4 (2) | C1—N3—C2—N5 | 176.9 (3) |
| N1—Cu1—N6—C4 | 135 (2) | N6—N7—C3—N9 | -178.5 (3) |
| N1—Cu1—N6—N7 | -46 (2) | N6—N7—C3—N8 | -0.3 (3) |
| C4—N6—N7—C3 | 0.5 (3) | C4—N8—C3—N9 | 178.2 (3) |
| Cu1—N6—N7—C3 | -178.76 (19) | C4—N8—C3—N7 | 0.0 (3) |
| N1—N2—C1—N4 | 179.3 (3) | N7—N6—C4—N10 | -177.9 (3) |
| N1—N2—C1—N3 | -0.2 (4) | Cu1—N6—C4—N10 | 1.2 (5) |
| C2—N3—C1—N2 | 0.9 (3) | N7—N6—C4—N8 | -0.5 (3) |
| C2—N3—C1—N4 | -178.6 (3) | Cu1—N6—C4—N8 | 178.6 (2) |
| N2—N1—C2—N5 | -177.0 (3) | C3—N8—C4—N6 | 0.3 (3) |
| Cu1—N1—C2—N5 | 9.7 (5) | C3—N8—C4—N10 | 177.8 (3) |

Symmetry code: (i) $-x+2, -y, -z$.

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|----------|-------------|-------------|---------------|
| N2—H2 \cdots F2 ⁱⁱ | 0.86 (2) | 1.86 (2) | 2.694 (3) | 166 (4) |
| N3—H3 \cdots F8 | 0.88 (2) | 2.02 (3) | 2.798 (3) | 146 (4) |
| N4—H4B \cdots F1 ⁱⁱⁱ | 0.86 | 1.95 | 2.742 (4) | 153 |
| N4—H4A \cdots F9 ⁱⁱⁱ | 0.86 | 1.95 | 2.801 (3) | 171 |
| N5—H5A \cdots F6 ^{iv} | 0.86 | 1.95 | 2.803 (3) | 174 |
| N5—H5B \cdots F9 ⁱ | 0.86 | 2.07 | 2.898 (3) | 162 |
| N7—H7 \cdots F4 ⁱⁱ | 0.86 (2) | 1.85 (2) | 2.686 (3) | 162 (4) |
| N8—H8 \cdots F7 ^v | 0.86 (2) | 2.04 (3) | 2.812 (3) | 148 (4) |
| N8—H8 \cdots F3 ^v | 0.86 (2) | 2.22 (3) | 2.813 (3) | 126 (3) |
| N9—H9B \cdots F8 ^{vi} | 0.86 | 2.05 | 2.892 (3) | 166 |
| N9—H9A \cdots F5 ^{vii} | 0.86 | 2.02 | 2.841 (4) | 159 |
| N10—H10B \cdots F5 ^v | 0.86 | 2.22 | 2.909 (3) | 137 |
| N10—H10A \cdots F6 ^{iv} | 0.86 | 2.02 | 2.845 (3) | 160 |

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $x-1, y, z$; (iii) $-x+1, -y+1, -z$; (iv) $x, y-1, z$; (v) $-x+1, -y, -z+1$; (vi) $x-1, y, z+1$; (vii) $-x, -y+1, -z+1$.