

## Hydrogen-bonded frameworks of bis(2-carboxypyridinium) hexafluorosilicate and bis(2-carboxyquinolinium) hexafluorosilicate dihydrate

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Received 26 May 2007

Accepted 19 July 2007

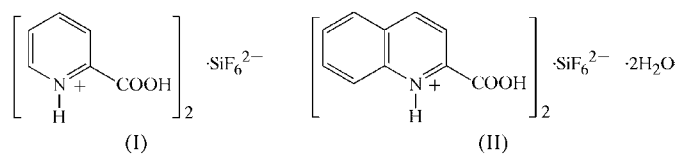
Online 9 August 2007

In bis(2-carboxypyridinium) hexafluorosilicate,  $2C_6H_6NO_2^+ \cdot SiF_6^{2-}$ , (I), and bis(2-carboxyquinolinium) hexafluorosilicate dihydrate,  $2C_{10}H_8NO_2^+ \cdot SiF_6^{2-} \cdot 2H_2O$ , (II), the Si atoms of the anions reside on crystallographic centres of inversion. Primary inter-ion interactions in (I) occur *via* strong N—H...F and O—H...F hydrogen bonds, generating corrugated layers incorporating  $[SiF_6]^{2-}$  anions as four-connected net nodes and organic cations as simple links in between. In (II), a set of strong N—H...F, O—H...O and O—H...F hydrogen bonds, involving water molecules, gives a three-dimensional hetero-coordinated rutile-like framework that integrates  $[SiF_6]^{2-}$  anions as six-connected and water molecules as three-connected nodes. The carboxyl groups of the cation are hydrogen bonded to the water molecule [O...O = 2.5533 (13) Å], while the N—H group supports direct bonding to the anion [N...F = 2.7061 (12) Å].

### Comment

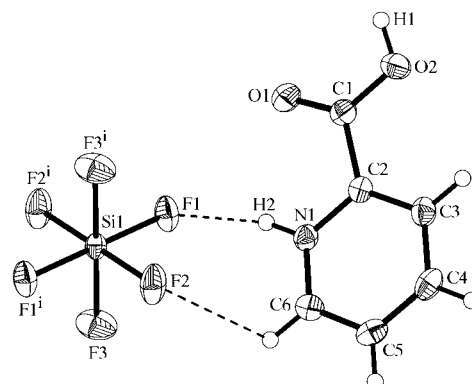
Fluorosilicate salts involving onium cations of N- and O-containing organic bases have practical applications as ionic liquids (Katayama *et al.*, 2001), dielectrics with cryptocrystal-line structure (Kalem, 2004), layered organic–inorganic hybrid materials (Airoldi & De Farias, 2000) and chemical reagents (Han *et al.*, 2000; Gelmboldt, 1989). Their structure is commonly dominated by strong directional interactions involving F atoms and convenient hydrogen-bond donors, although the relationships in such systems could be more complicated due to the presence of competitive OH and NH binding sites, inclusion of solvent molecules and extensive weak C—H...F hydrogen bonding, as occurs for 4-carboxyanilinium hexafluorosilicate hydrate (Gelmboldt *et al.*, 2004). Therefore, heteroaromatic onium cations combining sets of

typical hydrogen-bond donating functions (such as  $NH^+$ , COOH,  $CONH_2$ , *etc.*) are especially well suited for the examination of the hydrogen-bonding preferences of  $[SiF_6]^{2-}$  and are useful as rigid building blocks for the design of framework structures. In this context, we have prepared two new  $[SiF_6]^{2-}$  salts involving the cations 2-carboxypyridinium and 2-carboxyquinolinium as ambidentate N—H/O—H hydrogen-bond donors, giving the title compounds, (I) and (II), respectively, and report their structures here.



Compounds (I) and (II) adopt complicated framework structures originating in strong hydrogen bonding between the cationic and anionic counterparts. In (I), the  $[SiF_6]^{2-}$  anion is centrosymmetric, with the Si atom occupying a crystallographic centre of inversion (Fig. 1). Each of the 2-carboxypyridinium cations provides a pair of strong directional hydrogen bonds (N—H...F and O—H...F) (Table 2). This is a second known example of direct hydrogen bonding of a carboxyl group to  $[SiF_6]^{2-}$ ; the O...F separations in (I) and in the *N*-carboxymethyl-*N*-methylpiperidinium salt (2.58 and 2.56 Å, respectively; Szafran *et al.*, 2001) are similar. Thus, the  $[SiF_6]^{2-}$  anion accepts (in total) two pairs of such interactions utilizing four F atoms, which are coplanar within the coordination octahedron. Therefore, the primary strong hydrogen-bond connectivity in the structure may be considered as a plane (4,4) net, with  $[SiF_6]^{2-}$  anions providing four-connected net nodes and with the organic cations as simple links between them (Fig. 2). Such a principle is comparable with the eight-connected framework topology of tetrakis(2-carboxypyridinium)octacyanomolybdate(IV) (Basson *et al.*, 1980) and this suggests the utility of the bifunctional organic cations in the design of hydrogen-bonded frameworks, in combination with suitable counter-anions as geometrically rigid acceptors of hydrogen bonds.

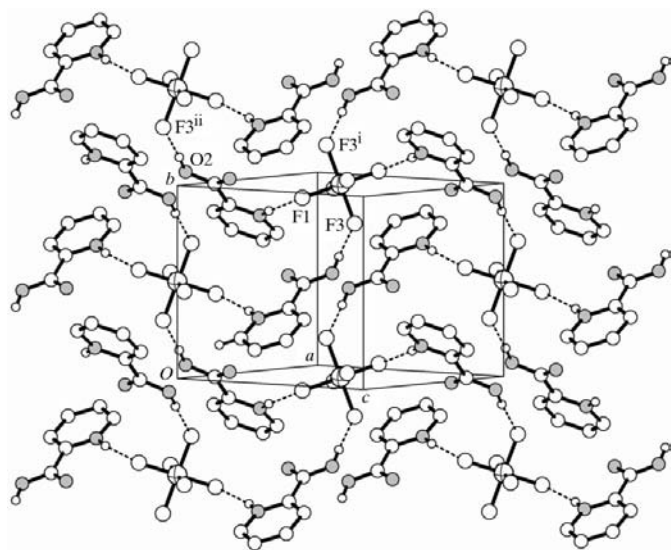
Corrugated hydrogen-bonded layers of (I) are parallel to the  $[101]$  plane and pack with a set of weaker interlayer



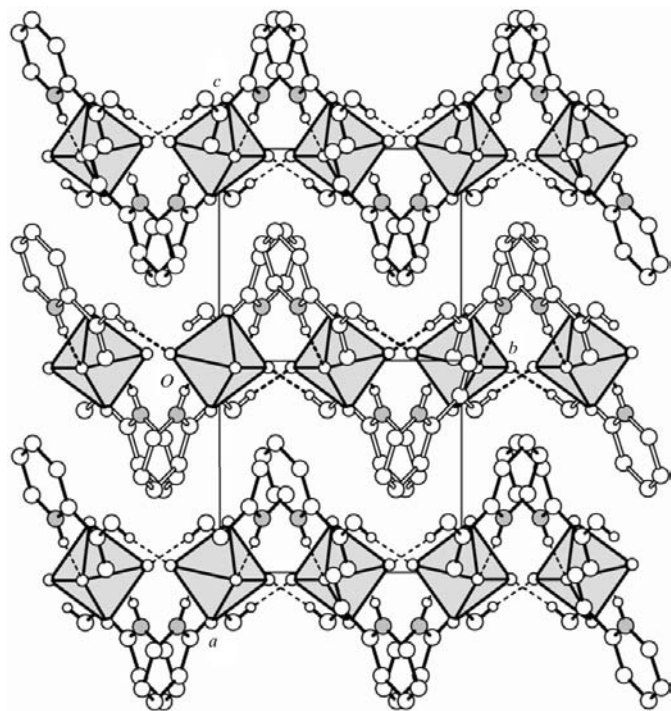
**Figure 1**

A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry code: (i)  $1 - x, 2 - y, 1 - z$ .]

interactions (Fig. 3), such as C—H···F hydrogen bonding ( $C\cdots F = 3.14\text{--}3.18\text{ \AA}$ ; Table 2) and a weak slipped  $\pi\text{--}\pi$  interaction that occurs between a pair of antiparallel organic moieties related by inversion (symmetry code:  $1 - x, 2 - y, -z$ ). The parameters of such interactions, *i.e.* the interplanar and intercentroid distances [ $3.347(2)$  and  $3.626(1)\text{ \AA}$ ,



**Figure 2**  
A view of the O—H···F and N—H···F hydrogen-bonded four-connected network in (I). [Symmetry codes: (i)  $1 - x, 2 - y, 1 - z$ ; (ii)  $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ .]



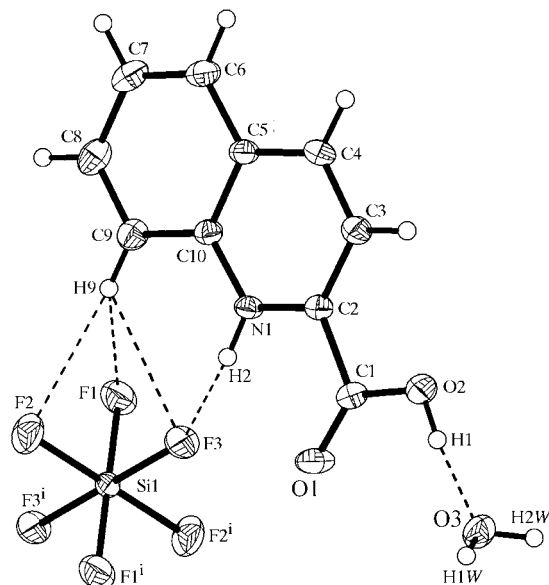
**Figure 3**  
A projection of the structure of (I) onto the  $[101]$  plane, showing the packing mode of three successive hydrogen-bonded layers. The  $[\text{SiF}_6]^{2-}$  anions are represented as shaded polyhedra.

respectively] and the slippage angle [ $22.6(1)^\circ$ ], are typical for  $\pi\text{--}\pi$  contacts between electron-deficient heteroaromatic rings (Janiak, 2000).

In the quinolinium salt, (II), the Si atom of the anion resides on an inversion centre (Fig. 4). The structure is more complicated due to the incorporation of water molecules, which provide additional donor and acceptor sites for strong hydrogen bonding. This is the first structure involving simple 2-carboxyquinolinium cations, since in the previously reported salts of 3-carboxy-4-hydroxybenzenesulfonate (Smith *et al.*, 2004), iodocuprate (Goher *et al.*, 2001) and tetrabromoaurate (Goher *et al.*, 1994), the 2-carboxyquinolinium cations were typically associated by strong O—H···O hydrogen bonding with neutral zwitterionic quinolinium-2-carboxylate moieties.

The carboxyl group of (II) donates a strong hydrogen bond to the O atom of the water molecule (Table 4), while the N—H function interacts directly with the  $[\text{SiF}_6]^{2-}$  anions, similar to (I). This situation parallels the hydrogen-bonding preferences of the anion in 4-carboxyanilinium hexafluorosilicate hydrate (Gelmboldt *et al.*, 2004), while in a simpler hydrated quinolinium salt, the cation–anion interaction was extended by inclusion of water molecules (N—H···OH<sub>2</sub>···F; Conley *et al.*, 2002). Here, the incorporation of water molecules indicates a lack of convenient hydrogen-bond donors for the quinolinium/ $[\text{SiF}_6]^{2-}$  system in (II).

The water molecules of (II) form pairs of O—H···F bonds with the anions [ $O\cdots F = 2.6707(13)$  and  $2.7070(13)\text{ \AA}$ ], in a very characteristic manner found for aqua–anion dimers (Domasevitch & Boldog, 2005). This generates aqua–anion chains along the *a*-axis direction in the crystal structure (Fig. 5) and the organic cations connect these chains into a three-



**Figure 4**  
A view of (II), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Dashed lines indicate hydrogen bonds. Note the trifurcated hydrogen bonding of the C9—H9 group. [Symmetry code: (i)  $-x, 2 - y, -z$ .]

dimensional framework as simple bitopic connectors (using O—H and N—H functions). Thus, either F atom of the anions accepts one strong hydrogen bond and the water molecule participates in three such interactions as an acceptor of one and donor of two bonds. Therefore, the entire hydrogen-bonded structure exists as a three-dimensional heterocoordinated framework consisting of three- (water molecules) and six-connected ( $[\text{SiF}_6]^{2-}$  anions) nodes in the ratio 2:1 (total Schlaffi symbol  $\{4;6^2\}2\{4^2;6^{10};8^3\}$ ) (Fig. 6). Such topology is commonly related to the heterocoordinated rutile net (rtl) (O’Keeffe *et al.*, 2000).

There are weaker hydrogen bonds involving the aromatic C—H groups of (II), in particular the C9—H9 group directed towards the F1/F2/F3 triangular edge of the  $[\text{SiF}_6]$  octahedron, forming a trifurcated hydrogen bond (Fig. 4). Stacking interactions are also of significance for the crystal packing. These occur between the carbocyclic ring of the cation and two carboxyl groups situated on both axial sides (Fig. 7). Atoms O1<sup>v</sup> and O2<sup>vi</sup> [symmetry codes: (v)  $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ ; (vi)  $-\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ ] are situated almost exactly above the ring centroid with relatively short O...centroid distances (3.22 and 3.30 Å) (Table 5). Such stacking may be compared with recently documented examples of  $\pi$ ...anion (heteroatom) interactions, which are characteristic for the most electron-deficient systems of 1,2,4,5-tetrazine (Schottel *et al.*, 2006) and 1,3,5-triazine (Maheswari *et al.*, 2006) [ $\text{F}(\text{O})\cdots\pi = 2.80$ – $3.20$  Å].

In both structures, the organic cations adopt a planar structure [O1—C1—C2—N1 torsion angles do not exceed  $-3.3$  (2)°], with a *trans* orientation of the O—H and N—H

groups. The geometric parameters agree well with those of the 2-carboxypyridinium (Smith *et al.*, 1995) and 2-carboxyquinolinium salts (Goher *et al.*, 2001).

The geometry of the  $[\text{SiF}_6]^{2-}$  anion is sensitive to  $\text{H}\cdots\text{F}$  hydrogen bonding and strong interactions effect an elongation of some Si—F bonds. This is observed in (I) and involves a set of three main bond types (O—H...F3, N—H...F1 and C—H...F2), with a longest Si—F separation corresponding to the F atom interacting with the strongest hydrogen-bond donor [ $\text{Si}-\text{F}3 = 1.7003$  (9) Å; Table 1]. For (II), there is no such evident differentiation in the strength of the primary hydrogen bonding (N—H...F and O—H...F with water molecules) and all three unique Si—F separations are similar (Table 3).

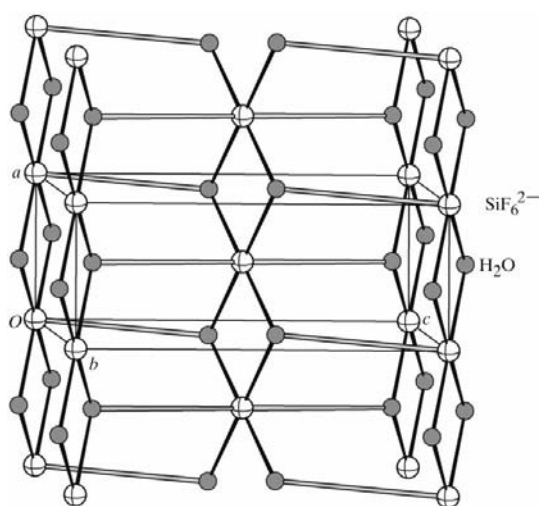


Figure 6

A schematic view of the heterocoordinated three-dimensional rutile-like framework topology in (II). The long grey-shaded links of the net represent 2-carboxyquinolinium bridges between  $[\text{SiF}_6]^{2-}$  anions (six-connected nodes) and water molecules (three-connected nodes).

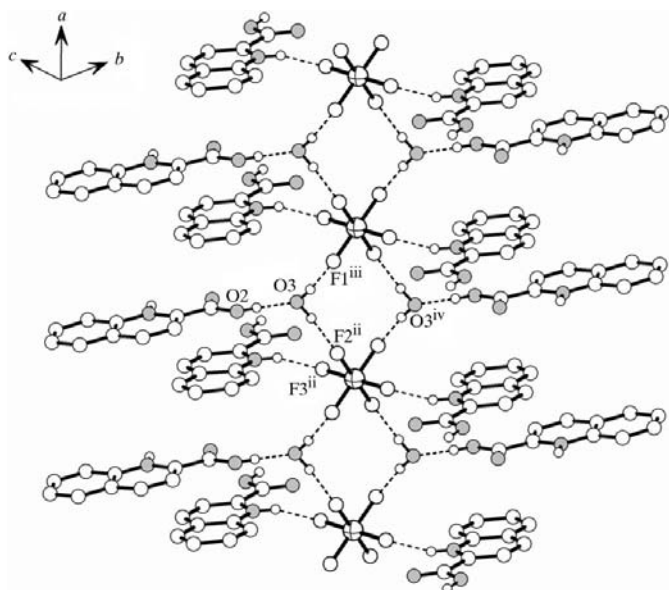


Figure 5

A view of the aqua- $[\text{SiF}_6]^{2-}$  chains dominating the connectivity in the structure of (II). The  $[\text{SiF}_6]^{2-}$  anion (acceptor of six hydrogen bonds) and the water molecules (acceptors of one and donors of two hydrogen bonds) provide six- and three-connected net nodes for the entire three-dimensional framework. [Symmetry codes: (ii)  $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ ; (iii)  $-\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ ; (iv)  $-x, 3 - y, 1 - z$ .]

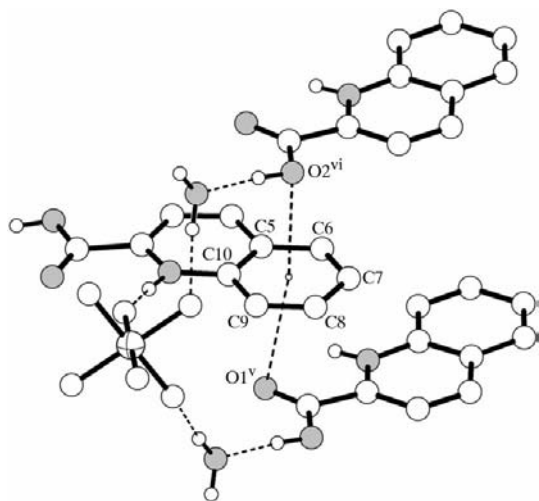


Figure 7

Stacking interactions between the carbocyclic fragment and two carboxyl groups of the 2-carboxyquinolinium cations in (II). [Symmetry codes: (v)  $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ ; (vi)  $-\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ .]

In conclusion, both 2-carboxypyridinium and 2-carboxyquinolinium cations reveal potential as singly charged donors of two strong hydrogen bonds and, in combination with  $[\text{SiF}_6]^{2-}$ , they support two- and three-dimensional framework topologies.

## Experimental

Compounds (I) and (II) were obtained as large colourless prisms by crystallization of pyridine-2- and quinoline-2-carboxylic acids from aqueous methanolic hexafluorosilicic acid by slow evaporation of the solutions at room temperature. In a typical synthesis, pyridine-2-carboxylic acid (0.123 g, 1 mmol) was dissolved in methanol (3 ml) under reflux and this solution was combined with 45% aqueous  $\text{H}_2\text{SiF}_6$  (0.9 ml, molar ratio 1:3). The reaction mixture was allowed to stand at room temperature until colourless transparent crystals were deposited (m.p. 455 K, without decomposition).

### Compound (I)

#### Crystal data

$2\text{C}_6\text{H}_6\text{NO}_2^+\cdot\text{SiF}_6^{2-}$   $V = 721.81 (11) \text{ \AA}^3$   
 $M_r = 390.33$   $Z = 2$   
 Monoclinic,  $P2_1/n$  Mo  $K\alpha$  radiation  
 $a = 9.3571 (9) \text{ \AA}$   $\mu = 0.26 \text{ mm}^{-1}$   
 $b = 7.8717 (6) \text{ \AA}$   $T = 173 (2) \text{ K}$   
 $c = 9.8053 (8) \text{ \AA}$   $0.17 \times 0.16 \times 0.14 \text{ mm}$   
 $\beta = 91.943 (7)^\circ$

#### Data collection

Stoe IPDS diffractometer 1646 reflections with  $I > 2\sigma(I)$   
 9005 measured reflections  $R_{\text{int}} = 0.059$   
 1935 independent reflections

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$  115 parameters  
 $wR(F^2) = 0.092$  H-atom parameters constrained  
 $S = 1.04$   $\Delta\rho_{\text{max}} = 0.39 \text{ e \AA}^{-3}$   
 1935 reflections  $\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ) for (I).

Si1—F1	1.6866 (8)	O2—C1	1.3147 (17)
Si1—F2	1.6621 (8)	N1—C2	1.3453 (16)
Si1—F3	1.7003 (9)	N1—C6	1.3349 (17)
O1—C1	1.2015 (17)	C1—C2	1.5047 (17)
F1—Si1—F2	90.73 (4)	O1—C1—O2	126.77 (13)
F1—Si1—F3	90.08 (5)	O1—C1—C2	121.01 (12)
F2—Si1—F3	90.15 (6)	O2—C1—C2	112.19 (11)
O2—C1—C2—C3	−1.22 (18)		

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ) for (I).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H1 $\cdots$ F3 <sup>i</sup>	0.85	1.76	2.5819 (14)	163
N1—H2 $\cdots$ F1	0.88	1.85	2.6730 (14)	156
C3—H3 $\cdots$ F2 <sup>ii</sup>	0.95	2.37	3.1785 (18)	142
C5—H5 $\cdots$ F1 <sup>iii</sup>	0.95	2.36	3.1364 (15)	139
C5—H5 $\cdots$ F2 <sup>iv</sup>	0.95	2.56	3.4602 (16)	159
C6—H6 $\cdots$ F2	0.95	2.61	3.0416 (17)	108

Symmetry codes: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $-x + 1, -y + 2, -z$ ; (iii)  $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$ ; (iv)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ .

### Compound (II)

#### Crystal data

$2\text{C}_{10}\text{H}_8\text{NO}_2^+\cdot\text{SiF}_6^{2-}\cdot 2\text{H}_2\text{O}$   $V = 1067.57 (17) \text{ \AA}^3$   
 $M_r = 526.47$   $Z = 2$   
 Monoclinic,  $P2_1/n$  Mo  $K\alpha$  radiation  
 $a = 6.6382 (6) \text{ \AA}$   $\mu = 0.21 \text{ mm}^{-1}$   
 $b = 9.4274 (9) \text{ \AA}$   $T = 173 (2) \text{ K}$   
 $c = 17.0668 (14) \text{ \AA}$   $0.16 \times 0.12 \times 0.12 \text{ mm}$   
 $\beta = 91.731 (8)^\circ$

#### Data collection

Stoe IPDS diffractometer 2368 reflections with  $I > 2\sigma(I)$   
 9457 measured reflections  $R_{\text{int}} = 0.039$   
 2697 independent reflections

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$  160 parameters  
 $wR(F^2) = 0.102$  H-atom parameters constrained  
 $S = 1.05$   $\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$   
 2697 reflections  $\Delta\rho_{\text{min}} = -0.42 \text{ e \AA}^{-3}$

**Table 3**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ) for (II).

Si1—F1	1.6830 (8)	N1—C10	1.3718 (14)
Si1—F2	1.6861 (8)	O1—C1	1.2061 (15)
Si1—F3	1.6834 (7)	O2—C1	1.3086 (15)
N1—C2	1.3349 (14)	C1—C2	1.5065 (15)
F1—Si1—F2	89.74 (5)	O1—C1—O2	127.59 (11)
F1—Si1—F3	89.59 (4)	O1—C1—C2	120.95 (11)
F2—Si1—F3	90.19 (4)	O2—C1—C2	111.45 (10)
O1—C1—C2—N1	−1.58 (19)		

**Table 4**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ) for (II).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H2 $\cdots$ F3	0.88	1.86	2.7061 (12)	160
O2—H1 $\cdots$ O3	0.85	1.71	2.5531 (13)	171
O3—H1W $\cdots$ F2 <sup>i</sup>	0.85	1.86	2.7070 (13)	175
O3—H2W $\cdots$ F1 <sup>ii</sup>	0.85	1.82	2.6707 (13)	176
C3—H3 $\cdots$ F2 <sup>iii</sup>	0.95	2.63	3.2125 (15)	120
C4—H4 $\cdots$ O3 <sup>iv</sup>	0.95	2.51	3.3940 (15)	156
C4—H4 $\cdots$ F2 <sup>iii</sup>	0.95	2.69	3.2526 (15)	118
C6—H6 $\cdots$ O1 <sup>iv</sup>	0.95	2.43	3.1655 (16)	134
C7—H7 $\cdots$ F1 <sup>v</sup>	0.95	2.59	3.3463 (16)	137
C9—H9 $\cdots$ F1	0.95	2.59	3.3823 (15)	141
C9—H9 $\cdots$ F2	0.95	2.57	3.4900 (16)	164
C9—H9 $\cdots$ F3	0.95	2.62	3.2907 (15)	128

Symmetry codes: (i)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $-x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (iii)  $x - \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$ ; (iv)  $x, y - 1, z$ ; (v)  $-x, -y + 1, -z$ .

**Table 5**

Carbonyl $\cdots\pi$  contacts ( $\text{\AA}$ ,  $^\circ$ ) for (II).

For details, see Fig. 7.  $\varphi$  is the angle of the  $\text{O}\cdots\pi$  axis with respect to the plane of the aromatic ring.

O atom	$\text{C}\cdots\text{O}$ range	$\text{O}\cdots\pi$	$\text{O}\cdots\text{plane}$	$\varphi$
O1 <sup>v</sup>	3.31–3.71	3.2240 (11)	3.1830 (13)	80.9 (2)
O2 <sup>vi</sup>	3.40–3.77	3.3008 (11)	3.2626 (13)	81.3 (2)

Symmetry codes: (v)  $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ ; (vi)  $-\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$ .

All H atoms were located in difference maps and then treated as riding, with O–H distances constrained to 0.85 Å, N–H distances constrained to 0.88 Å and C–H distances constrained to 0.95 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{N,O})$ .

For both compounds, data collection: *IPDS Software* (Stoe & Cie, 2000); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Version 1.700.00; Farrugia, 1999).

The authors acknowledge support from the Deutsche Forschungsgemeinschaft (KVD).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GG3102). Services for accessing these data are described at the back of the journal.

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