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A new polymorph of 1,3-bis(pentafluorophenyl)urea

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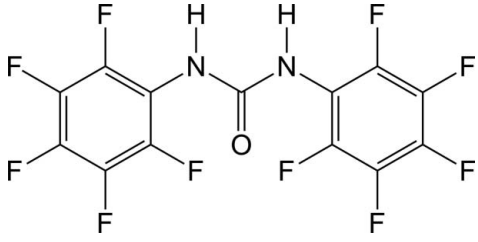
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.080; data-to-parameter ratio = 8.3.

The title compound, $C_{13}H_2F_{10}N_2O$, has been previously described in the space group *Pbca* with Z = 8 [Jai-nhuknan *et al.* (1997). *Acta Cryst.* C**53**, 455–457]. The current $P2_12_12_1$ polymorph was obtained from a tetrahydrofuran solution. The pentafluorophenyl rings make dihedral angles of 50.35 (6) and 54.94 (6)° with the urea fragment, in close accord with those reported for the first polymorph. In the crystal, both of the N—H groups donate H atoms to the same carbonyl O atom, forming a one-dimensional molecular array along the *a* axis. There are close contacts between perfluorophenyl C atoms within the array [3.228 (3) Å] and halogen bonds are also observed between the arrays [F···F = 2.709 (2) and 2.7323 (18) Å].

Related literature

For the structure of the first reported ploymorph, see: Jai-nhuknan *et al.* (1997). For the related structure of 1,3-diphenylurea, see: Dannecker *et al.* (1979). For background to organofluorine chemistry, see: Chambers (2004).



Experimental

Crystal data

$C_{13}H_2F_{10}N_2O$
M_r = 392.16
Orthorhombic, $P2_12_12_1$
a = 4.5798 (7) Å
b = 9.5411 (16) Å
c = 29.136 (5) Å
V = 1273.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 93 K
0.15 × 0.15 × 0.03 mm

Data collection

Rigaku Saturn724+ diffractometer
Absorption correction: numerical (*NUMABS*; Rigaku, 1999)
T_{min} = 0.978, T_{max} = 0.993
10307 measured reflections
1993 independent reflections
1941 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.080
S = 1.09
1991 reflections
241 parameters
2 restraints
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.864 (18)	2.057 (18)	2.850 (3)	152 (3)
N2—H2···O1^{i}	0.879 (18)	2.008 (18)	2.825 (3)	154 (3)

Symmetry code: (i) $x+1, y, z$.

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR92* (Altomare, *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2101).

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supporting information

Acta Cryst. (2013). E**69**, o608 [doi:10.1107/S1600536813007836]

A new polymorph of 1,3-bis(pentafluorophenyl)urea

Tsunehisa Okuno

S1. Comment

Perfluoro aromatic compounds have attracted interest from the viewpoint of the electronic and structural comparison with the original compounds (Chambers, 2004). The title compound, (I), is a perfluoro compound of 1,3-diphenylurea (Dannecker *et al.*, 1979). Previously, (I) was isolated in an orthorhombic *Pbca* polymorph with $Z = 8$ [Jai-nhuknan *et al.*, 1997]. A new orthorhombic $P2_12_12_1$ polymorph was obtained by recrystallization from a tetrahydrofuran solution.

The dihedral angle between the C1—C6/F1—F5 (r.m.s. deviation = 0.0223 Å) and the C7—C12/F6—F10 (r.m.s. deviation = 0.0181 Å) pentafluorophenyl rings is 30.93 (3)°, which is smaller than that of the reported polymorph. The pentafluorophenyl rings make dihedral angles of 50.35 (6)° and 54.94 (6)°, respectively, with the C13/N1/N2/O1 urea fragment (r.m.s. deviation = 0.0011 Å), and this situation is almost accordance with the reported polymorph.

Both of the N—H groups in one molecule donate protons to the same carbonyl O atom, forming a one-dimensional molecular array along the *a* axis, where the N···O distances were 2.850 (3) Å for N1···O1^{i} and 2.825 (3) Å for N2···O1^{i} [Symmetry code: (i) $x + 1, y, z$] (Figure 2). There are close contacts between perfluorophenyl carbons within the array, where the C2···C5^{i} distance is 3.228 (3) Å. Halogen-bonds are also recognized between the arrays. The distances of F2···F10^{ii} and F1···F5^{iii} are 2.709 (2) Å and 2.7323 (18) Å, respectively [Symmetry codes: (ii) $-x + 1, y + 1/2, -z + 1/2$ (iii) $-x + 2, y + 1/2, -z + 1/2$.] (Figure 2).

S2. Experimental

The title compound was commercially purchased and recrystallized from a tetrahydrofuran solution.

S3. Refinement

Friedel pairs were merged because the molecule itself was achiral and because there were not any anomalous scattering effects. The N-bound H atom was obtained from a difference Fourier map and was refined isotropically with the restriction of N—H range between 0.85 Å and 0.89 Å. U_{iso}(H) values of the H atoms were set at $1.2U_{eq}$(parent atom).

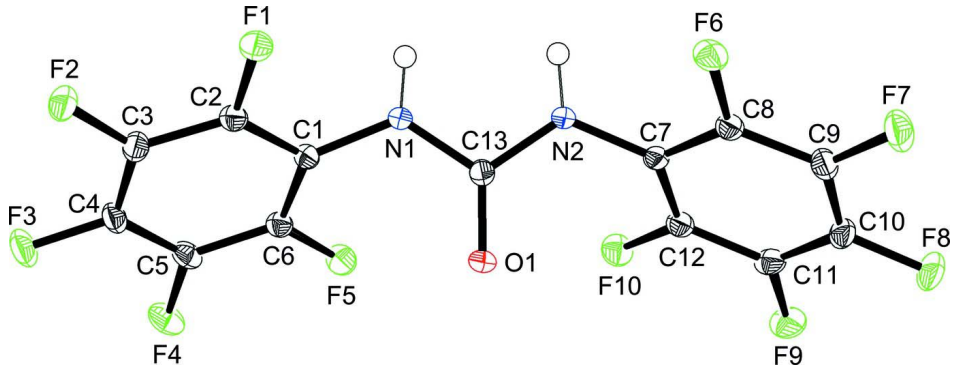

Figure 1

The asymmetric unit of the title compound with atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres.

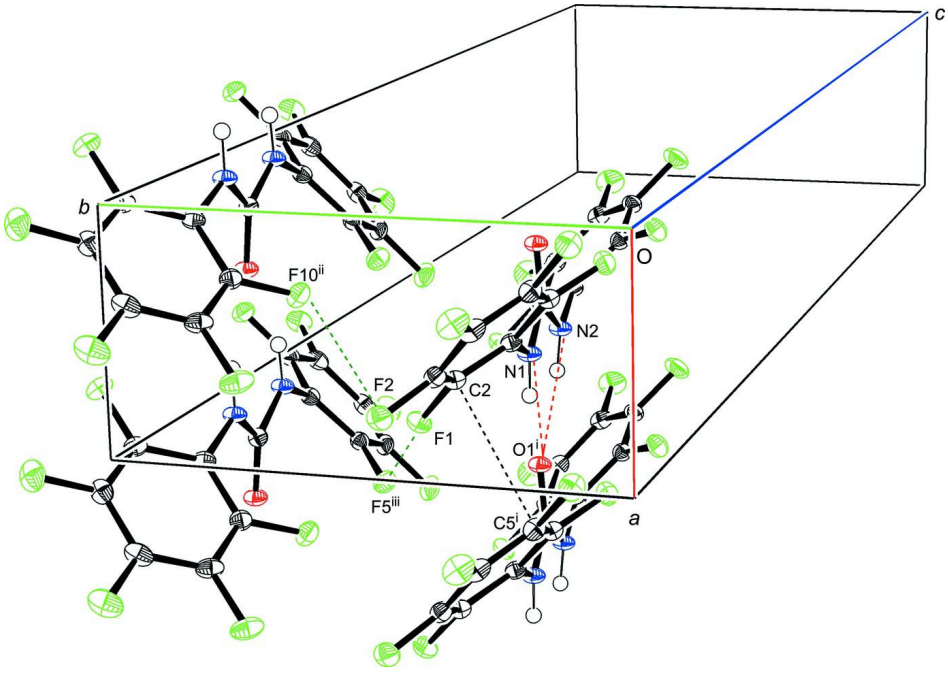

Figure 2

A view of the intermolecular interactions in the title compound. [Symmetry codes: (i) $x + 1, y, z$ (ii) $-x + 1, y + 1/2, -z + 1/2$ (iii)$-x + 2, y + 1/2, -z + 1/2$.]

1,3-Bis(pentafluorophenyl)urea

Crystal data

$C_{13}H_2F_{10}N_2O$
$M_r = 392.16$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.5798$ (7) Å
$b = 9.5411$ (16) Å
$c = 29.136$ (5) Å
$V = 1273.1$ (4) Å^3
$Z = 4$

$F(000) = 768.00$
$D_x = 2.046$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 4650 reflections
$\theta = 2.3$–$31.2°$
$\mu = 0.23$ mm^{-1}
$T = 93$ K
Platelet, colorless
0.15 × 0.15 × 0.03 mm

Data collection

Rigaku Saturn724+ diffractometer
Detector resolution: 28.445 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Rigaku, 1999)
T_{min} = 0.978, T_{max} = 0.993
10307 measured reflections
1993 independent reflections
1941 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.023
θ_{max} = 29.0°
h = −6→5
k = −12→13
l = −39→37

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.080
S = 1.09
1991 reflections
241 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 0.6807P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections except for two with very negative F^2. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating R-factor (gt).

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

	x	y	z	U_{iso}*/U_{eq}
F1	1.1418 (3)	0.61873 (13)	0.20307 (4)	0.0201 (3)
F2	0.9729 (3)	0.60115 (14)	0.11485 (4)	0.0230 (3)
F3	0.5296 (4)	0.42251 (14)	0.09057 (4)	0.0261 (3)
F4	0.2849 (3)	0.25518 (13)	0.15527 (4)	0.0235 (3)
F5	0.4741 (3)	0.26032 (12)	0.24218 (4)	0.0199 (3)
F6	1.1205 (3)	0.65289 (13)	0.41004 (4)	0.0209 (3)
F7	0.9048 (4)	0.66890 (14)	0.49612 (4)	0.0269 (3)
F8	0.4722 (4)	0.49024 (15)	0.52340 (4)	0.0286 (3)
F9	0.2803 (3)	0.28817 (15)	0.46530 (4)	0.0261 (3)
F10	0.5071 (3)	0.26629 (12)	0.38011 (4)	0.0213 (3)
O1	0.4972 (3)	0.46701 (15)	0.30935 (5)	0.0163 (3)
N1	0.9286 (4)	0.4477 (2)	0.27009 (5)	0.0154 (3)
N2	0.9324 (4)	0.45284 (19)	0.34806 (5)	0.0149 (3)
C1	0.8112 (5)	0.4427 (2)	0.22555 (6)	0.0143 (4)
C2	0.9298 (5)	0.5288 (2)	0.19172 (6)	0.0156 (4)
C3	0.8433 (5)	0.5207 (2)	0.14616 (6)	0.0172 (4)
C4	0.6225 (5)	0.4295 (3)	0.13398 (6)	0.0180 (4)
C5	0.4991 (5)	0.3442 (2)	0.16699 (6)	0.0170 (4)
C6	0.5947 (5)	0.3492 (2)	0.21201 (6)	0.0150 (4)
C7	0.8117 (4)	0.4624 (2)	0.39231 (6)	0.0141 (4)

C8	0.9103 (5)	0.5630 (2)	0.42307 (6)	0.0155 (4)
C9	0.8013 (5)	0.5723 (2)	0.46721 (6)	0.0181 (4)
C10	0.5852 (5)	0.4809 (3)	0.48127 (6)	0.0196 (4)
C11	0.4853 (5)	0.3785 (2)	0.45158 (6)	0.0184 (4)
C12	0.6005 (5)	0.3694 (2)	0.40767 (6)	0.0158 (4)
C13	0.7652 (5)	0.4563 (2)	0.30915 (6)	0.0139 (4)
H1	1.117 (4)	0.451 (3)	0.2722 (9)	0.0184*
H2	1.123 (4)	0.459 (3)	0.3452 (9)	0.0179*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0170 (6)	0.0229 (6)	0.0204 (6)	−0.0048 (5)	−0.0003 (5)	−0.0012 (5)
F2	0.0234 (6)	0.0297 (6)	0.0158 (5)	0.0024 (6)	0.0033 (5)	0.0049 (5)
F3	0.0296 (7)	0.0353 (7)	0.0135 (5)	0.0054 (7)	−0.0075 (6)	−0.0045 (5)
F4	0.0220 (6)	0.0210 (6)	0.0276 (6)	−0.0030 (6)	−0.0094 (6)	−0.0061 (5)
F5	0.0200 (6)	0.0195 (6)	0.0202 (6)	−0.0027 (6)	−0.0016 (5)	0.0030 (5)
F6	0.0185 (6)	0.0226 (6)	0.0215 (6)	−0.0072 (6)	−0.0018 (5)	0.0029 (5)
F7	0.0326 (8)	0.0299 (7)	0.0181 (5)	−0.0002 (7)	−0.0049 (6)	−0.0073 (5)
F8	0.0303 (7)	0.0426 (8)	0.0129 (5)	0.0047 (7)	0.0060 (6)	0.0026 (5)
F9	0.0201 (6)	0.0324 (7)	0.0259 (6)	−0.0066 (6)	0.0043 (6)	0.0104 (6)
F10	0.0221 (6)	0.0197 (6)	0.0221 (6)	−0.0056 (6)	−0.0011 (5)	−0.0017 (5)
O1	0.0100 (6)	0.0234 (7)	0.0154 (6)	−0.0001 (6)	−0.0011 (6)	0.0006 (6)
N1	0.0097 (7)	0.0242 (8)	0.0122 (7)	0.0003 (7)	−0.0006 (6)	−0.0007 (6)
N2	0.0094 (7)	0.0237 (8)	0.0117 (7)	0.0000 (7)	−0.0004 (6)	0.0004 (6)
C1	0.0126 (8)	0.0174 (8)	0.0129 (8)	0.0016 (8)	−0.0009 (7)	−0.0011 (7)
C2	0.0134 (8)	0.0178 (8)	0.0155 (8)	0.0009 (7)	−0.0004 (7)	−0.0017 (7)
C3	0.0180 (9)	0.0202 (9)	0.0135 (8)	0.0046 (8)	0.0014 (7)	0.0013 (7)
C4	0.0193 (9)	0.0230 (9)	0.0116 (8)	0.0063 (9)	−0.0036 (8)	−0.0040 (7)
C5	0.0159 (9)	0.0165 (8)	0.0186 (8)	0.0001 (8)	−0.0051 (8)	−0.0043 (7)
C6	0.0136 (8)	0.0163 (8)	0.0152 (8)	0.0015 (8)	−0.0007 (7)	−0.0010 (7)
C7	0.0111 (8)	0.0184 (9)	0.0127 (8)	0.0013 (8)	−0.0003 (7)	0.0026 (7)
C8	0.0134 (8)	0.0180 (8)	0.0151 (8)	−0.0005 (8)	−0.0008 (7)	0.0026 (7)
C9	0.0197 (9)	0.0200 (9)	0.0147 (8)	0.0027 (8)	−0.0029 (8)	−0.0017 (7)
C10	0.0190 (9)	0.0277 (10)	0.0122 (8)	0.0060 (9)	0.0015 (7)	0.0032 (7)
C11	0.0141 (8)	0.0224 (9)	0.0188 (8)	0.0003 (8)	0.0015 (8)	0.0081 (7)
C12	0.0139 (8)	0.0172 (8)	0.0162 (8)	0.0003 (8)	−0.0012 (7)	0.0010 (7)
C13	0.0141 (8)	0.0150 (8)	0.0126 (8)	−0.0006 (7)	−0.0003 (7)	0.0000 (7)

Geometric parameters (Å, º)

F1—C2	1.337 (3)	C1—C2	1.393 (3)
F2—C3	1.332 (3)	C1—C6	1.391 (3)
F3—C4	1.336 (3)	C2—C3	1.387 (3)
F4—C5	1.342 (3)	C3—C4	1.380 (3)
F5—C6	1.340 (3)	C4—C5	1.381 (3)
F6—C8	1.344 (3)	C5—C6	1.384 (3)
F7—C9	1.336 (3)	C7—C8	1.389 (3)

F8—C10	1.335 (3)	C7—C12	1.387 (3)
F9—C11	1.336 (3)	C8—C9	1.382 (3)
F10—C12	1.340 (3)	C9—C10	1.381 (3)
O1—C13	1.232 (3)	C10—C11	1.383 (3)
N1—C1	1.405 (3)	C11—C12	1.387 (3)
N1—C13	1.364 (3)	N1—H1	0.864 (18)
N2—C7	1.406 (3)	N2—H2	0.879 (18)
N2—C13	1.368 (3)		

F1···F2	2.6895 (18)	F9···C11^{xiv}	3.197 (3)
F1···N1	2.725 (2)	F10···F1^{vi}	3.2313 (18)
F2···F3	2.744 (2)	F10···F2^{viii}	2.709 (2)
F3···F4	2.7126 (18)	F10···F2^{vi}	2.859 (2)
F4···F5	2.6767 (18)	F10···F3^{viii}	3.3936 (19)
F5···O1	2.7803 (19)	F10···N2^{v}	3.312 (3)
F5···N1	2.862 (3)	F10···C3^{viii}	2.942 (3)
F5···C13	3.014 (3)	F10···C4^{viii}	3.293 (3)
F6···F7	2.6999 (18)	O1···F4^{i}	3.101 (2)
F6···N2	2.765 (2)	O1···F5^{i}	3.1785 (19)
F7···F8	2.732 (2)	O1···N1^{v}	2.850 (3)
F8···F9	2.712 (2)	O1···N2^{v}	2.825 (3)
F9···F10	2.6989 (18)	O1···C13^{v}	3.354 (3)
F10···O1	2.8143 (19)	N1···F1^{vi}	3.251 (3)
F10···N2	2.799 (3)	N1···F5^{iii}	3.178 (3)
F10···C13	2.993 (3)	N1···F5^{i}	3.525 (3)
O1···C1	2.843 (3)	N1···O1^{iii}	2.850 (3)
O1···C6	3.083 (3)	N2···F1^{vi}	3.535 (3)
O1···C7	2.814 (3)	N2···F2^{vi}	3.552 (3)
O1···C12	3.049 (3)	N2···F4^{i}	3.053 (3)
C1···C4	2.807 (3)	N2···F10^{iii}	3.312 (3)
C2···C5	2.741 (3)	N2···O1^{iii}	2.825 (3)
C2···C13	3.571 (3)	C1···F1^{v}	3.557 (3)
C3···C6	2.767 (3)	C1···F4^{iii}	3.478 (3)
C6···C13	3.109 (3)	C1···F5^{iii}	3.532 (3)
C7···C10	2.797 (3)	C1···F5^{i}	3.432 (3)
C8···C11	2.753 (3)	C2···F4^{iii}	3.254 (3)
C8···C13	3.535 (3)	C2···F5^{i}	3.466 (3)
C9···C12	2.757 (3)	C2···C5^{iii}	3.228 (3)
C12···C13	3.082 (3)	C2···C6^{iii}	3.544 (3)
F1···F5^{i}	3.5106 (18)	C3···F4^{iii}	3.252 (3)
F1···F5^{ii}	2.7323 (18)	C3···F10^{i}	2.942 (3)
F1···F10^{ii}	3.2313 (18)	C3···C5^{iii}	3.496 (3)
F1···N1^{ii}	3.251 (3)	C4···F1^{v}	3.487 (3)
F1···N2^{ii}	3.535 (3)	C4···F2^{v}	3.441 (3)
F1···C1^{iii}	3.557 (3)	C4···F4^{iii}	3.515 (3)
F1···C4^{iii}	3.487 (3)	C4···F6^{vi}	3.162 (3)
F1···C5^{iii}	3.263 (3)	C4···F10^{i}	3.293 (3)
F1···C6^{iii}	3.315 (3)	C5···F1^{v}	3.263 (3)

F1···C6^{ii}	3.523 (3)	C5···F6^{vi}	3.377 (3)
F1···C13^{ii}	3.269 (3)	C5···C2^{v}	3.228 (3)
F2···F3^{iii}	3.147 (2)	C5···C3^{v}	3.496 (3)
F2···F8^{iv}	2.8148 (18)	C6···F1^{v}	3.315 (3)
F2···F9^{i}	3.1594 (19)	C6···F1^{vi}	3.523 (3)
F2···F10^{i}	2.709 (2)	C6···C2^{v}	3.544 (3)
F2···F10^{ii}	2.859 (2)	C7···F2^{vi}	3.591 (3)
F2···N2^{ii}	3.552 (3)	C7···F4^{i}	3.150 (3)
F2···C4^{iii}	3.441 (3)	C7···F9^{iii}	3.448 (3)
F2···C7^{ii}	3.591 (3)	C8···F4^{i}	3.061 (3)
F2···C12^{ii}	3.286 (3)	C8···F9^{iii}	3.356 (3)
F3···F2^{v}	3.147 (2)	C8···C11^{iii}	3.275 (3)
F3···F6^{vi}	3.0309 (19)	C9···F7^{xi}	3.246 (3)
F3···F7^{iv}	2.9024 (18)	C9···F8^{iii}	3.568 (3)
F3···F8^{vii}	3.131 (2)	C9···F9^{iii}	3.487 (3)
F3···F8^{iv}	3.119 (2)	C10···F6^{v}	3.395 (3)
F3···F10^{i}	3.3936 (19)	C10···F7^{xi}	3.504 (3)
F4···F6^{viii}	2.8319 (18)	C10···F9^{xiii}	3.133 (3)
F4···F6^{vi}	3.4627 (19)	C11···F6^{v}	3.333 (3)
F4···O1^{viii}	3.101 (2)	C11···F9^{xiii}	3.197 (3)
F4···N2^{viii}	3.053 (3)	C11···C8^{v}	3.275 (3)
F4···C1^{v}	3.478 (3)	C12···F2^{vi}	3.286 (3)
F4···C2^{v}	3.254 (3)	C12···F6^{v}	3.486 (3)
F4···C3^{v}	3.252 (3)	C13···F1^{vi}	3.269 (3)
F4···C4^{v}	3.515 (3)	C13···F4^{i}	3.043 (3)
F4···C7^{viii}	3.150 (3)	C13···F5^{i}	3.442 (3)
F4···C8^{viii}	3.061 (3)	C13···O1^{iii}	3.354 (3)
F4···C13^{viii}	3.043 (3)	F1···H1	2.58 (3)
F5···F1^{viii}	3.5106 (18)	F5···H1	3.57 (2)
F5···F1^{vi}	2.7323 (18)	F6···H2	2.64 (3)
F5···O1^{viii}	3.1785 (19)	F10···H2	3.52 (3)
F5···N1^{v}	3.178 (3)	O1···H1	3.040 (19)
F5···N1^{viii}	3.525 (3)	O1···H2	3.052 (19)
F5···C1^{v}	3.532 (3)	N1···H2	2.37 (3)
F5···C1^{viii}	3.432 (3)	N2···H1	2.37 (3)
F5···C2^{viii}	3.466 (3)	C2···H1	2.61 (3)
F5···C13^{viii}	3.442 (3)	C6···H1	3.12 (3)
F6···F3^{ii}	3.0309 (19)	C8···H2	2.66 (3)
F6···F4^{i}	2.8319 (18)	C12···H2	3.13 (3)
F6···F4^{ii}	3.4627 (19)	H1···H2	2.13 (4)
F6···F7^{ix}	3.4730 (18)	F1···H1^{ii}	3.46 (3)
F6···C4^{ii}	3.162 (3)	F4···H2^{viii}	3.39 (3)
F6···C5^{ii}	3.377 (3)	F5···H1^{v}	2.60 (3)
F6···C10^{iii}	3.395 (3)	F5···H1^{vi}	3.52 (3)
F6···C11^{iii}	3.333 (3)	F10···H2^{v}	2.74 (3)
F6···C12^{iii}	3.486 (3)	O1···H1^{v}	2.06 (2)
F7···F3^{x}	2.9024 (18)	O1···H2^{v}	2.01 (2)
F7···F6^{xi}	3.4730 (18)	C1···H1^{v}	3.460 (19)

F7···F7^{xi}	2.773 (2)	C6···H1^{v}	2.97 (3)
F7···F7^{ix}	2.773 (2)	C7···H2^{v}	3.44 (2)
F7···F8^{iii}	3.208 (3)	C11···H2^{v}	3.60 (3)
F7···F8^{ix}	3.316 (2)	C12···H2^{v}	2.97 (3)
F7···C9^{ix}	3.246 (3)	C13···H1^{v}	3.160 (19)
F7···C10^{ix}	3.504 (3)	C13···H2^{v}	3.123 (19)
F8···F2^{x}	2.8148 (18)	H1···F1^{vi}	3.46 (3)
F8···F3^{xii}	3.131 (2)	H1···F5^{iii}	2.60 (3)
F8···F3^{x}	3.119 (2)	H1···F5^{ii}	3.52 (3)
F8···F7^{v}	3.208 (3)	H1···O1^{iii}	2.06 (2)
F8···F7^{xi}	3.316 (2)	H1···C1^{iii}	3.460 (19)
F8···F9^{xiii}	3.026 (2)	H1···C6^{iii}	2.97 (3)
F8···C9^{v}	3.568 (3)	H1···C13^{iii}	3.160 (19)
F9···F2^{viii}	3.1594 (19)	H2···F4^{i}	3.39 (3)
F9···F8^{xiv}	3.026 (2)	H2···F10^{iii}	2.74 (3)
F9···F9^{xiv}	3.1405 (19)	H2···O1^{iii}	2.01 (2)
F9···F9^{xiii}	3.1405 (19)	H2···C7^{iii}	3.44 (2)
F9···C7^{v}	3.448 (3)	H2···C11^{iii}	3.60 (3)
F9···C8^{v}	3.356 (3)	H2···C12^{iii}	2.97 (3)
F9···C9^{v}	3.487 (3)	H2···C13^{iii}	3.123 (19)
F9···C10^{xiv}	3.133 (3)		

C1—N1—C13	124.23 (17)	F6—C8—C7	119.45 (16)
C7—N2—C13	122.57 (16)	F6—C8—C9	118.75 (17)
N1—C1—C2	118.94 (18)	C7—C8—C9	121.79 (19)
N1—C1—C6	123.82 (17)	F7—C9—C8	120.16 (19)
C2—C1—C6	117.09 (17)	F7—C9—C10	120.19 (17)
F1—C2—C1	119.10 (16)	C8—C9—C10	119.65 (18)
F1—C2—C3	118.66 (17)	F8—C10—C9	120.58 (18)
C1—C2—C3	122.19 (18)	F8—C10—C11	119.58 (19)
F2—C3—C2	119.74 (18)	C9—C10—C11	119.84 (17)
F2—C3—C4	120.90 (16)	F9—C11—C10	120.09 (17)
C2—C3—C4	119.36 (18)	F9—C11—C12	120.21 (17)
F3—C4—C3	120.55 (18)	C10—C11—C12	119.70 (19)
F3—C4—C5	119.96 (19)	F10—C12—C7	119.93 (16)
C3—C4—C5	119.49 (17)	F10—C12—C11	118.52 (18)
F4—C5—C4	119.68 (17)	C7—C12—C11	121.54 (18)
F4—C5—C6	119.63 (17)	O1—C13—N1	123.73 (17)
C4—C5—C6	120.70 (19)	O1—C13—N2	123.75 (17)
F5—C6—C1	120.90 (16)	N1—C13—N2	112.52 (17)
F5—C6—C5	118.00 (17)	C1—N1—H1	116.7 (17)
C1—C6—C5	121.09 (18)	C13—N1—H1	119.0 (17)
N2—C7—C8	120.58 (17)	C7—N2—H2	118.2 (17)
N2—C7—C12	121.92 (17)	C13—N2—H2	118.4 (17)
C8—C7—C12	117.45 (17)		

C1—N1—C13—O1	−3.5 (3)	F4—C5—C6—F5	2.1 (3)
C1—N1—C13—N2	177.01 (17)	F4—C5—C6—C1	−178.37 (15)

C13—N1—C1—C2	133.29 (19)	C4—C5—C6—F5	−177.65 (17)
C13—N1—C1—C6	−51.4 (3)	C4—C5—C6—C1	1.8 (3)
C7—N2—C13—O1	−0.5 (3)	N2—C7—C8—F6	0.8 (3)
C7—N2—C13—N1	179.00 (16)	N2—C7—C8—C9	−178.16 (16)
C13—N2—C7—C8	−125.94 (19)	N2—C7—C12—F10	0.4 (3)
C13—N2—C7—C12	56.8 (3)	N2—C7—C12—C11	179.16 (16)
N1—C1—C2—F1	−3.3 (3)	C8—C7—C12—F10	−176.99 (16)
N1—C1—C2—C3	174.14 (16)	C8—C7—C12—C11	1.8 (3)
N1—C1—C6—F5	3.0 (3)	C12—C7—C8—F6	178.23 (16)
N1—C1—C6—C5	−176.48 (16)	C12—C7—C8—C9	−0.8 (3)
C2—C1—C6—F5	178.43 (16)	F6—C8—C9—F7	−0.1 (3)
C2—C1—C6—C5	−1.1 (3)	F6—C8—C9—C10	179.98 (15)
C6—C1—C2—F1	−178.95 (16)	C7—C8—C9—F7	178.88 (17)
C6—C1—C2—C3	−1.5 (3)	C7—C8—C9—C10	−1.0 (3)
F1—C2—C3—F2	0.4 (3)	F7—C9—C10—F8	1.7 (3)
F1—C2—C3—C4	−179.26 (15)	F7—C9—C10—C11	−178.09 (17)
C1—C2—C3—F2	−177.03 (17)	C8—C9—C10—F8	−178.41 (18)
C1—C2—C3—C4	3.3 (3)	C8—C9—C10—C11	1.8 (3)
F2—C3—C4—F3	−1.5 (3)	F8—C10—C11—F9	−1.1 (3)
F2—C3—C4—C5	177.88 (16)	F8—C10—C11—C12	179.42 (16)
C2—C3—C4—F3	178.15 (17)	C9—C10—C11—F9	178.72 (18)
C2—C3—C4—C5	−2.5 (3)	C9—C10—C11—C12	−0.8 (3)
F3—C4—C5—F4	−0.4 (3)	F9—C11—C12—F10	−1.8 (3)
F3—C4—C5—C6	179.35 (16)	F9—C11—C12—C7	179.43 (16)
C3—C4—C5—F4	−179.83 (18)	C10—C11—C12—F10	177.76 (17)
C3—C4—C5—C6	−0.0 (3)	C10—C11—C12—C7	−1.0 (3)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+2, *y*+1/2, −*z*+1/2; (iii) *x*+1, *y*, *z*; (iv) −*x*+3/2, −*y*+1, *z*−1/2; (v) *x*−1, *y*, *z*; (vi) −*x*+2, *y*−1/2, −*z*+1/2; (vii) −*x*+1/2, −*y*+1, *z*−1/2; (viii) −*x*+1, *y*−1/2, −*z*+1/2; (ix) *x*+1/2, −*y*+3/2, −*z*+1; (x) −*x*+3/2, −*y*+1, *z*+1/2; (xi) *x*−1/2, −*y*+3/2, −*z*+1; (xii) −*x*+1/2, −*y*+1, *z*+1/2; (xiii) *x*+1/2, −*y*+1/2, −*z*+1; (xiv) *x*−1/2, −*y*+1/2, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{iii}	0.864 (18)	2.057 (18)	2.850 (3)	152 (3)
N2—H2···O1^{iii}	0.879 (18)	2.008 (18)	2.825 (3)	154 (3)

Symmetry code: (iii) *x*+1, *y*, *z*.