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Supporting information for article:

Twist-chair conformation of the tetraoxepane ring remains unchanged in tetraoxaspirododecane diamines

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Computing details

For all compounds, data collection: *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01); cell refinement: *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01); data reduction: *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01). Program(s) used to solve structure: ShelXT (Sheldrick, 2015) for compound_I, compound_III; *SHELXD* (Sheldrick, 2008) for compound_II. For all compounds, program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: Olex2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: Olex2 (Dolomanov *et al.*, 2009).

(compound_I)

Crystal data

$C_{20}H_{22}Cl_2N_2O_4$	$F(000)$ = 888
M_r = 425.30	D_x = 1.413 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 10.5362 (9) Å	Cell parameters from 3198 reflections
b = 9.4705 (6) Å	θ = 2.4–26.8°
c = 20.3165 (17) Å	μ = 0.35 mm^{-1}
β = 99.462 (8)°	T = 293 K
V = 1999.7 (3) Å^3	Prizm
Z = 4	0.72 × 0.54 × 0.28 mm

Data collection

Xcalibur, Eos diffractometer	4644 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2780 reflections with $I > 2\sigma(I)$
Graphite monochromator	R_{int} = 0.045
Detector resolution: 16.1709 pixels mm^{-1}	θ_{max} = 29.3°, θ_{min} = 2.0°
ω scans	h = -12→14
Absorption correction: multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	k = -12→12
T_{min} = 0.647, T_{max} = 1.000	l = -24→27

13245 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.059$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.188$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} < 0.001$
4644 reflections	$\Delta\rangle_{max} = 0.36$ e Å^{-3}
261 parameters	$\Delta\rangle_{min} = -0.31$ e Å^{-3}
0 restraints	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (compound_I)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1040 (3)	0.4237 (3)	0.60376 (12)	0.0401 (6)
C2	0.1259 (3)	0.3086 (3)	0.55582 (14)	0.0539 (8)
H2A	0.217624	0.295086	0.557512	0.065*
H2B	0.089375	0.336911	0.510797	0.065*
C3	0.0650 (4)	0.1692 (3)	0.57237 (18)	0.0659 (10)
H3A	0.073075	0.100386	0.537937	0.079*
H3B	0.110618	0.133207	0.614374	0.079*
C4	-0.0753 (4)	0.1878 (3)	0.57741 (19)	0.0733 (11)
H4A	-0.110567	0.098182	0.588783	0.088*
H4B	-0.122083	0.217472	0.534494	0.088*
C5	-0.0928 (3)	0.2964 (3)	0.62969 (17)	0.0634 (9)
H5A	-0.051376	0.263888	0.673234	0.076*
H5B	-0.183754	0.308703	0.630992	0.076*
C6	-0.0343 (3)	0.4371 (3)	0.61351 (15)	0.0508 (7)
H6A	-0.084610	0.475530	0.573215	0.061*
H6B	-0.039275	0.503006	0.649541	0.061*

C9	0.3026 (3)	0.6716 (3)	0.64838 (13)	0.0407 (6)
H9	0.349226	0.669286	0.610449	0.049*
C10	0.3503 (2)	0.5515 (3)	0.69623 (13)	0.0404 (6)
H10	0.318660	0.564717	0.738561	0.048*
C14	0.3664 (2)	0.9212 (3)	0.65061 (13)	0.0397 (6)
C15	0.4270 (3)	1.0295 (3)	0.69015 (14)	0.0471 (7)
H15	0.433712	1.023756	0.736289	0.057*
C16	0.4768 (3)	1.1441 (3)	0.66243 (15)	0.0529 (8)
H16	0.518498	1.214611	0.689677	0.063*
C17	0.4653 (3)	1.1551 (3)	0.59440 (14)	0.0477 (7)
C18	0.4018 (3)	1.0541 (3)	0.55388 (14)	0.0519 (7)
H18	0.391895	1.063502	0.507751	0.062*
C19	0.3518 (3)	0.9370 (3)	0.58200 (14)	0.0489 (7)
H19	0.308095	0.868413	0.554381	0.059*
C21	0.5605 (2)	0.4661 (3)	0.75524 (13)	0.0406 (6)
C22	0.5104 (3)	0.3963 (3)	0.80536 (13)	0.0434 (6)
H22	0.423220	0.403803	0.807575	0.052*
C23	0.5890 (3)	0.3160 (3)	0.85179 (14)	0.0461 (7)
H23	0.555368	0.270577	0.885680	0.055*
C24	0.7169 (3)	0.3036 (3)	0.84774 (14)	0.0458 (7)
C25	0.7681 (3)	0.3704 (3)	0.79841 (16)	0.0592 (8)
H25	0.854873	0.360056	0.795724	0.071*
C26	0.6904 (3)	0.4527 (3)	0.75295 (15)	0.0571 (8)
H26	0.725529	0.500175	0.720132	0.068*
Cl1	0.53118 (9)	1.30125 (9)	0.56012 (5)	0.0733 (3)
Cl2	0.81568 (8)	0.19855 (9)	0.90578 (4)	0.0632 (3)
N13	0.3226 (2)	0.8028 (2)	0.68056 (13)	0.0469 (6)
H13	0.337 (3)	0.808 (3)	0.7198 (14)	0.039 (8)*
N20	0.4854 (2)	0.5511 (3)	0.70745 (13)	0.0465 (6)
H20	0.518 (3)	0.569 (4)	0.6770 (16)	0.061 (11)*
O7	0.15156 (19)	0.54649 (18)	0.57565 (9)	0.0490 (5)
O8	0.16622 (18)	0.66138 (18)	0.62410 (10)	0.0480 (5)
O11	0.31096 (17)	0.41454 (17)	0.66852 (9)	0.0433 (5)
O12	0.17285 (16)	0.40240 (18)	0.66976 (8)	0.0416 (4)

Atomic displacement parameters (Å²) for (compound_I)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0413 (14)	0.0399 (13)	0.0367 (13)	0.0000 (11)	-0.0001 (11)	0.0035 (11)
C2	0.0571 (19)	0.0555 (17)	0.0467 (16)	0.0022 (13)	0.0019 (14)	-0.0062 (13)

C3	0.076 (2)	0.0455 (16)	0.071 (2)	0.0005 (15)	-0.0035 (18)	-0.0075 (14)
C4	0.073 (3)	0.0568 (19)	0.080 (2)	-0.0175 (16)	-0.016 (2)	0.0101 (17)
C5	0.0493 (19)	0.070 (2)	0.069 (2)	-0.0101 (15)	0.0038 (15)	0.0122 (17)
C6	0.0429 (15)	0.0549 (16)	0.0514 (16)	0.0039 (13)	-0.0018 (13)	0.0030 (13)
C9	0.0389 (15)	0.0410 (14)	0.0431 (14)	0.0013 (11)	0.0094 (11)	-0.0003 (11)
C10	0.0353 (14)	0.0417 (14)	0.0443 (14)	-0.0013 (11)	0.0071 (11)	-0.0037 (11)
C14	0.0342 (14)	0.0386 (13)	0.0458 (14)	0.0052 (10)	0.0051 (11)	-0.0012 (11)
C15	0.0510 (17)	0.0451 (15)	0.0445 (15)	0.0015 (12)	0.0057 (12)	-0.0082 (12)
C16	0.0539 (18)	0.0408 (14)	0.0619 (19)	-0.0025 (13)	0.0033 (14)	-0.0082 (13)
C17	0.0460 (16)	0.0430 (14)	0.0537 (17)	0.0012 (12)	0.0069 (13)	0.0025 (12)
C18	0.0564 (18)	0.0549 (16)	0.0435 (15)	0.0015 (14)	0.0054 (13)	0.0008 (13)
C19	0.0509 (17)	0.0433 (14)	0.0503 (16)	-0.0023 (12)	0.0011 (13)	-0.0045 (12)
C21	0.0347 (14)	0.0391 (13)	0.0469 (14)	-0.0040 (11)	0.0037 (11)	-0.0045 (11)
C22	0.0308 (13)	0.0468 (14)	0.0535 (15)	-0.0028 (11)	0.0092 (11)	-0.0027 (12)
C23	0.0405 (16)	0.0500 (15)	0.0478 (15)	-0.0032 (12)	0.0076 (12)	-0.0008 (12)
C24	0.0379 (15)	0.0454 (15)	0.0512 (16)	-0.0011 (11)	-0.0009 (12)	-0.0042 (12)
C25	0.0286 (14)	0.074 (2)	0.076 (2)	0.0010 (14)	0.0090 (14)	0.0115 (16)
C26	0.0368 (16)	0.0696 (19)	0.0661 (19)	-0.0047 (14)	0.0124 (14)	0.0166 (15)
Cl1	0.0760 (6)	0.0635 (5)	0.0804 (6)	-0.0202 (4)	0.0132 (5)	0.0081 (4)
Cl2	0.0546 (5)	0.0749 (5)	0.0570 (5)	0.0137 (4)	0.0000 (4)	0.0065 (4)
N13	0.0570 (16)	0.0424 (13)	0.0422 (14)	-0.0049 (10)	0.0108 (11)	-0.0035 (11)
N20	0.0349 (13)	0.0562 (14)	0.0490 (14)	-0.0006 (10)	0.0084 (11)	0.0085 (11)
O7	0.0572 (12)	0.0463 (10)	0.0410 (10)	-0.0055 (9)	0.0004 (9)	0.0043 (8)
O8	0.0413 (11)	0.0405 (10)	0.0605 (12)	0.0048 (8)	0.0031 (9)	0.0006 (8)
O11	0.0325 (10)	0.0436 (10)	0.0528 (11)	0.0020 (8)	0.0041 (8)	-0.0020 (8)
O12	0.0343 (10)	0.0488 (10)	0.0399 (10)	-0.0015 (8)	0.0009 (7)	0.0031 (8)

Geometric parameters (Å, º) for (compound_I)

C1—C2	1.505 (4)	C14—N13	1.390 (3)
C1—C6	1.508 (4)	C15—H15	0.9300
C1—O7	1.423 (3)	C15—C16	1.367 (4)
C1—O12	1.430 (3)	C16—H16	0.9300
C2—H2A	0.9700	C16—C17	1.371 (4)
C2—H2B	0.9700	C17—C18	1.364 (4)
C2—C3	1.529 (4)	C17—Cl1	1.744 (3)
C3—H3A	0.9700	C18—H18	0.9300
C3—H3B	0.9700	C18—C19	1.389 (4)
C3—C4	1.508 (5)	C19—H19	0.9300
C4—H4A	0.9700	C21—C22	1.389 (4)

C4—H4B	0.9700	C21—C26	1.383 (4)
C4—C5	1.511 (5)	C21—N20	1.401 (3)
C5—H5A	0.9700	C22—H22	0.9300
C5—H5B	0.9700	C22—C23	1.377 (4)
C5—C6	1.526 (4)	C23—H23	0.9300
C6—H6A	0.9700	C23—C24	1.368 (4)
C6—H6B	0.9700	C24—C25	1.369 (4)
C9—H9	0.9800	C24—Cl2	1.749 (3)
C9—C10	1.527 (3)	C25—H25	0.9300
C9—N13	1.404 (3)	C25—C26	1.372 (4)
C9—O8	1.444 (3)	C26—H26	0.9300
C10—H10	0.9800	N13—H13	0.79 (3)
C10—N20	1.404 (3)	N20—H20	0.77 (4)
C10—O11	1.447 (3)	O7—O8	1.458 (2)
C14—C15	1.392 (3)	O11—O12	1.464 (2)
C14—C19	1.385 (4)		
C2—C1—C6	113.6 (2)	O11—C10—H10	109.9
O7—C1—C2	103.3 (2)	C19—C14—C15	117.7 (2)
O7—C1—C6	113.3 (2)	C19—C14—N13	122.6 (2)
O7—C1—O12	109.49 (18)	N13—C14—C15	119.7 (2)
O12—C1—C2	113.3 (2)	C14—C15—H15	119.4
O12—C1—C6	104.0 (2)	C16—C15—C14	121.2 (3)
C1—C2—H2A	109.3	C16—C15—H15	119.4
C1—C2—H2B	109.3	C15—C16—H16	120.0
C1—C2—C3	111.6 (3)	C15—C16—C17	119.9 (2)
H2A—C2—H2B	108.0	C17—C16—H16	120.0
C3—C2—H2A	109.3	C16—C17—Cl1	119.2 (2)
C3—C2—H2B	109.3	C18—C17—C16	120.6 (3)
C2—C3—H3A	109.3	C18—C17—Cl1	120.2 (2)
C2—C3—H3B	109.3	C17—C18—H18	120.2
H3A—C3—H3B	108.0	C17—C18—C19	119.5 (3)
C4—C3—C2	111.4 (3)	C19—C18—H18	120.2
C4—C3—H3A	109.3	C14—C19—C18	120.9 (2)
C4—C3—H3B	109.3	C14—C19—H19	119.5
C3—C4—H4A	109.4	C18—C19—H19	119.5
C3—C4—H4B	109.4	C22—C21—N20	122.8 (2)
C3—C4—C5	111.2 (3)	C26—C21—C22	118.6 (2)
H4A—C4—H4B	108.0	C26—C21—N20	118.6 (3)

C5—C4—H4A	109.4	C21—C22—H22	119.8
C5—C4—H4B	109.4	C23—C22—C21	120.5 (3)
C4—C5—H5A	109.7	C23—C22—H22	119.8
C4—C5—H5B	109.7	C22—C23—H23	120.2
C4—C5—C6	110.0 (3)	C24—C23—C22	119.6 (3)
H5A—C5—H5B	108.2	C24—C23—H23	120.2
C6—C5—H5A	109.7	C23—C24—C25	121.0 (2)
C6—C5—H5B	109.7	C23—C24—Cl2	119.4 (2)
C1—C6—C5	112.8 (2)	C25—C24—Cl2	119.6 (2)
C1—C6—H6A	109.0	C24—C25—H25	120.3
C1—C6—H6B	109.0	C24—C25—C26	119.5 (3)
C5—C6—H6A	109.0	C26—C25—H25	120.3
C5—C6—H6B	109.0	C21—C26—H26	119.5
H6A—C6—H6B	107.8	C25—C26—C21	120.9 (3)
C10—C9—H9	109.2	C25—C26—H26	119.5
N13—C9—H9	109.2	C9—N13—H13	121 (2)
N13—C9—C10	110.8 (2)	C14—N13—C9	123.0 (2)
N13—C9—O8	106.4 (2)	C14—N13—H13	112 (2)
O8—C9—H9	109.2	C10—N20—H20	116 (2)
O8—C9—C10	111.9 (2)	C21—N20—C10	123.8 (2)
C9—C10—H10	109.9	C21—N20—H20	114 (3)
N20—C10—C9	108.9 (2)	C1—O7—O8	110.13 (18)
N20—C10—H10	109.9	C9—O8—O7	105.63 (18)
N20—C10—O11	106.2 (2)	C10—O11—O12	106.58 (16)
O11—C10—C9	112.13 (19)	C1—O12—O11	109.00 (18)
C1—C2—C3—C4	53.1 (3)	C22—C21—N20—C10	-13.9 (4)
C1—O7—O8—C9	104.2 (2)	C22—C23—C24—C25	0.4 (4)
C2—C1—C6—C5	50.4 (3)	C22—C23—C24—Cl2	-178.7 (2)
C2—C1—O7—O8	-166.28 (19)	C23—C24—C25—C26	1.0 (5)
C2—C1—O12—O11	66.8 (3)	C24—C25—C26—C21	-1.7 (5)
C2—C3—C4—C5	-58.0 (4)	C26—C21—C22—C23	0.3 (4)
C3—C4—C5—C6	57.5 (3)	C26—C21—N20—C10	167.0 (3)
C4—C5—C6—C1	-53.5 (3)	Cl1—C17—C18—C19	178.8 (2)
C6—C1—C2—C3	-49.5 (3)	Cl2—C24—C25—C26	-180.0 (2)

C6—C1—O7—O8	70.3 (2)	N13—C9—C10—N20	-73.0 (3)
C6—C1—O12—O11	-169.39 (18)	N13—C9—C10—O11	169.8 (2)
C9—C10—N20—C21	171.7 (2)	N13—C9—O8—O7	164.42 (19)
C9—C10—O11—O12	-72.8 (2)	N13—C14—C15—C16	176.7 (3)
C10—C9—N13—C14	138.6 (3)	N13—C14—C19—C18	-177.2 (3)
C10—C9—O8—O7	-74.5 (2)	N20—C10—O11—O12	168.35 (19)
C10—O11—O12—C1	103.67 (19)	N20—C21—C22—C23	-178.9 (2)
C14—C15—C16—C17	1.3 (4)	N20—C21—C26—C25	-179.7 (3)
C15—C14—C19—C18	3.0 (4)	O7—C1—C2—C3	-172.7 (2)
C15—C14—N13—C9	-157.1 (3)	O7—C1—C6—C5	168.0 (2)
C15—C16—C17—C18	1.5 (5)	O7—C1—O12—O11	-48.0 (2)
C15—C16—C17—Cl1	-179.3 (2)	O8—C9—C10—N20	168.4 (2)
C16—C17—C18—C19	-2.0 (5)	O8—C9—C10—O11	51.2 (3)
C17—C18—C19—C14	-0.4 (4)	O8—C9—N13—C14	-99.5 (3)
C19—C14—C15—C16	-3.5 (4)	O11—C10—N20—C21	-67.4 (3)
C19—C14—N13—C9	23.2 (4)	O12—C1—C2—C3	68.9 (3)
C21—C22—C23—C24	-1.0 (4)	O12—C1—C6—C5	-73.2 (3)
C22—C21—C26—C25	1.1 (4)	O12—C1—O7—O8	-45.2 (2)

(compound_II)

Crystal data

$C_{20}H_{22}F_2N_2O_4$	$F(000)$ = 824
M_r = 392.40	D_x = 1.386 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 18.9061 (6) Å	Cell parameters from 2196 reflections
b = 11.4711 (4) Å	θ = 2.1–27.2°
c = 8.7831 (3) Å	μ = 0.11 mm^{-1}
β = 99.134 (3)°	T = 293 K
V = 1880.67 (11) Å^3	Prizm, colourless
Z = 4	0.52 × 0.32 × 0.29 mm

Data collection

Xcalibur, Eos diffractometer	4395 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2718 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.016$
Detector resolution: 16.1709 pixels mm^{-1}	$\theta_{max} = 29.2°$, $\theta_{min} = 2.1°$
ω scans	$h = -24 \rightarrow 17$
Absorption correction: multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	$k = -7 \rightarrow 15$
$T_{min} = 0.593$, $T_{max} = 1.000$	$l = -11 \rightarrow 9$
9078 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.162$	$w = 1/[\sigma^2(F_o^2) + (0.0675P)^2 + 0.4744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
4395 reflections	$\Delta\rangle_{max} = 0.21$ e $Å^{-3}$
261 parameters	$\Delta\rangle_{min} = -0.17$ e $Å^{-3}$
0 restraints	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for (compound_II)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.23777 (10)	0.02798 (17)	-0.0225 (2)	0.0369 (4)
C2	0.28211 (11)	-0.04452 (18)	-0.1160 (2)	0.0457 (5)

H2A	0.315454	0.005460	-0.158623	0.055*
H2B	0.250958	-0.081051	-0.201090	0.055*
C3	0.32325 (12)	-0.13764 (19)	-0.0161 (3)	0.0545 (6)
H3A	0.357973	-0.100672	0.062297	0.065*
H3B	0.349222	-0.185838	-0.079218	0.065*
C4	0.27386 (13)	-0.2140 (2)	0.0613 (3)	0.0605 (6)
H4A	0.242493	-0.257462	-0.016797	0.073*
H4B	0.302251	-0.269652	0.128259	0.073*
C5	0.22910 (13)	-0.1425 (2)	0.1548 (2)	0.0563 (6)
H5A	0.259943	-0.108501	0.242350	0.068*
H5B	0.194957	-0.192968	0.194093	0.068*
C6	0.18920 (11)	-0.04637 (19)	0.0589 (2)	0.0486 (5)
H6A	0.152393	-0.080860	-0.017277	0.058*
H6B	0.165665	0.002974	0.125347	0.058*
C9	0.20792 (10)	0.29987 (16)	-0.0555 (2)	0.0378 (4)
H9	0.210912	0.314805	-0.164192	0.045*
C10	0.28407 (10)	0.29235 (16)	0.0374 (2)	0.0379 (4)
H10	0.282083	0.305010	0.146988	0.045*
C14	0.11163 (10)	0.44631 (17)	-0.0831 (2)	0.0392 (5)
C15	0.09113 (11)	0.5549 (2)	-0.0374 (3)	0.0501 (5)
C16	0.03490 (13)	0.6159 (2)	-0.1168 (3)	0.0685 (7)
H16	0.022692	0.688800	-0.082704	0.082*
C17	-0.00332 (13)	0.5674 (3)	-0.2479 (3)	0.0716 (8)
H17	-0.041543	0.607759	-0.303745	0.086*
C18	0.01499 (12)	0.4597 (2)	-0.2960 (3)	0.0610 (6)
H18	-0.011045	0.427200	-0.384501	0.073*
C19	0.07163 (11)	0.3989 (2)	-0.2146 (2)	0.0479 (5)
H19	0.083118	0.325425	-0.248192	0.057*
C21	0.38551 (10)	0.42913 (17)	0.0805 (2)	0.0404 (5)
C22	0.41014 (11)	0.53715 (19)	0.0425 (3)	0.0482 (5)
C23	0.46557 (13)	0.5942 (2)	0.1310 (3)	0.0621 (6)
H23	0.480294	0.667047	0.101760	0.075*
C24	0.49904 (13)	0.5420 (3)	0.2635 (3)	0.0696 (7)
H24	0.536664	0.579540	0.325540	0.083*
C25	0.47673 (12)	0.4342 (2)	0.3042 (3)	0.0621 (6)
H25	0.499594	0.398805	0.394034	0.075*
C26	0.42087 (11)	0.3775 (2)	0.2138 (2)	0.0505 (5)
H26	0.406839	0.304043	0.242503	0.061*
F1	0.12913 (8)	0.60095 (12)	0.09316 (17)	0.0742 (4)

F2	0.37700 (8)	0.58683 (12)	-0.09048 (16)	0.0698 (4)
N13	0.17095 (9)	0.39167 (16)	0.0026 (2)	0.0455 (4)
H13	0.1811 (12)	0.409 (2)	0.094 (3)	0.056 (7)*
N20	0.32746 (10)	0.37810 (16)	-0.0150 (2)	0.0463 (4)
H20	0.3156 (13)	0.407 (2)	-0.103 (3)	0.070 (8)*
O7	0.19840 (7)	0.10592 (12)	-0.13077 (14)	0.0440 (4)
O8	0.16646 (7)	0.19510 (11)	-0.04342 (15)	0.0433 (4)
O11	0.31906 (7)	0.18243 (11)	0.01813 (15)	0.0427 (4)
O12	0.28075 (7)	0.09431 (11)	0.09484 (14)	0.0412 (3)

Atomic displacement parameters (Å²) for (compound_II)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0401 (10)	0.0365 (10)	0.0317 (9)	0.0008 (8)	-0.0014 (8)	-0.0021 (8)
C2	0.0547 (12)	0.0435 (12)	0.0402 (11)	0.0021 (10)	0.0113 (10)	-0.0013 (9)
C3	0.0562 (13)	0.0476 (13)	0.0593 (13)	0.0096 (11)	0.0077 (11)	-0.0013 (11)
C4	0.0800 (17)	0.0417 (12)	0.0592 (14)	0.0044 (12)	0.0089 (13)	0.0071 (11)
C5	0.0729 (15)	0.0517 (14)	0.0440 (12)	-0.0112 (12)	0.0084 (11)	0.0050 (11)
C6	0.0476 (11)	0.0501 (13)	0.0495 (12)	-0.0080 (10)	0.0119 (10)	-0.0047 (10)
C9	0.0377 (10)	0.0381 (10)	0.0365 (10)	0.0033 (8)	0.0023 (8)	-0.0005 (8)
C10	0.0350 (9)	0.0362 (10)	0.0403 (10)	0.0019 (8)	-0.0002 (8)	-0.0012 (8)
C14	0.0359 (10)	0.0404 (11)	0.0412 (10)	0.0026 (8)	0.0057 (8)	0.0051 (9)
C15	0.0427 (11)	0.0454 (12)	0.0605 (14)	0.0013 (10)	0.0029 (10)	-0.0003 (11)
C16	0.0594 (15)	0.0538 (15)	0.0914 (19)	0.0210 (12)	0.0092 (14)	0.0048 (14)
C17	0.0511 (14)	0.081 (2)	0.0780 (17)	0.0211 (13)	-0.0032 (13)	0.0235 (16)
C18	0.0459 (12)	0.0787 (18)	0.0541 (13)	0.0042 (12)	-0.0052 (10)	0.0096 (13)
C19	0.0438 (11)	0.0540 (13)	0.0438 (11)	0.0023 (10)	0.0007 (9)	0.0024 (10)
C21	0.0341 (10)	0.0391 (11)	0.0481 (11)	0.0001 (8)	0.0065 (9)	-0.0067 (9)
C22	0.0424 (11)	0.0433 (12)	0.0586 (13)	0.0013 (10)	0.0075 (10)	-0.0009 (11)
C23	0.0551 (14)	0.0498 (14)	0.0811 (18)	-0.0125 (11)	0.0094 (13)	-0.0090 (13)
C24	0.0520 (13)	0.0794 (19)	0.0739 (17)	-0.0161 (14)	-0.0007 (13)	-0.0204 (15)
C25	0.0482 (13)	0.0773 (18)	0.0562 (14)	0.0001 (12)	-0.0056 (11)	-0.0029 (13)
C26	0.0433 (11)	0.0530 (13)	0.0536 (12)	-0.0007 (10)	0.0030 (10)	0.0013 (11)
F1	0.0708 (9)	0.0568 (9)	0.0887 (10)	0.0090 (7)	-0.0065 (8)	-0.0228 (8)
F2	0.0733 (9)	0.0524 (8)	0.0791 (10)	-0.0037 (7)	-0.0019 (8)	0.0160 (7)
N13	0.0477 (10)	0.0473 (10)	0.0375 (9)	0.0125 (8)	-0.0053 (8)	-0.0075 (8)
N20	0.0467 (10)	0.0452 (10)	0.0440 (10)	-0.0092 (8)	-0.0019 (8)	0.0079 (9)
O7	0.0526 (8)	0.0401 (8)	0.0358 (7)	0.0047 (6)	-0.0036 (6)	-0.0052 (6)
O8	0.0372 (7)	0.0405 (8)	0.0510 (8)	0.0006 (6)	0.0037 (6)	-0.0046 (7)
O11	0.0366 (7)	0.0381 (8)	0.0532 (8)	0.0003 (6)	0.0067 (6)	0.0009 (6)

O12	0.0478 (8)	0.0372 (8)	0.0362 (7)	-0.0041 (6)	-0.0008 (6)	0.0013 (6)

Geometric parameters (Å, °) for (compound_II)

C1—C2	1.512 (3)	C14—N13	1.396 (2)
C1—C6	1.514 (3)	C15—C16	1.367 (3)
C1—O7	1.426 (2)	C15—F1	1.360 (2)
C1—O12	1.427 (2)	C16—H16	0.9300
C2—H2A	0.9700	C16—C17	1.376 (4)
C2—H2B	0.9700	C17—H17	0.9300
C2—C3	1.517 (3)	C17—C18	1.367 (4)
C3—H3A	0.9700	C18—H18	0.9300
C3—H3B	0.9700	C18—C19	1.379 (3)
C3—C4	1.518 (3)	C19—H19	0.9300
C4—H4A	0.9700	C21—C22	1.383 (3)
C4—H4B	0.9700	C21—C26	1.385 (3)
C4—C5	1.512 (3)	C21—N20	1.400 (3)
C5—H5A	0.9700	C22—C23	1.368 (3)
C5—H5B	0.9700	C22—F2	1.360 (2)
C5—C6	1.515 (3)	C23—H23	0.9300
C6—H6A	0.9700	C23—C24	1.371 (3)
C6—H6B	0.9700	C24—H24	0.9300
C9—H9	0.9800	C24—C25	1.373 (3)
C9—C10	1.541 (3)	C25—H25	0.9300
C9—N13	1.404 (2)	C25—C26	1.379 (3)
C9—O8	1.448 (2)	C26—H26	0.9300
C10—H10	0.9800	N13—H13	0.82 (2)
C10—N20	1.405 (2)	N20—H20	0.84 (2)
C10—O11	1.446 (2)	O7—O8	1.4652 (17)
C14—C15	1.383 (3)	O11—O12	1.4680 (17)
C14—C19	1.387 (3)		
C2—C1—C6	112.15 (18)	O11—C10—H10	109.5
O7—C1—C2	104.98 (14)	C15—C14—C19	117.00 (19)
O7—C1—C6	112.14 (15)	C15—C14—N13	119.06 (18)
O7—C1—O12	108.93 (15)	C19—C14—N13	123.93 (19)
O12—C1—C2	112.60 (15)	C16—C15—C14	122.9 (2)
O12—C1—C6	106.11 (14)	F1—C15—C14	117.39 (18)
C1—C2—H2A	109.5	F1—C15—C16	119.7 (2)
C1—C2—H2B	109.5	C15—C16—H16	120.6

C1—C2—C3	110.52 (16)	C15—C16—C17	118.8 (2)
H2A—C2—H2B	108.1	C17—C16—H16	120.6
C3—C2—H2A	109.5	C16—C17—H17	120.1
C3—C2—H2B	109.5	C18—C17—C16	119.9 (2)
C2—C3—H3A	109.3	C18—C17—H17	120.1
C2—C3—H3B	109.3	C17—C18—H18	119.6
C2—C3—C4	111.74 (19)	C17—C18—C19	120.7 (2)
H3A—C3—H3B	107.9	C19—C18—H18	119.6
C4—C3—H3A	109.3	C14—C19—H19	119.7
C4—C3—H3B	109.3	C18—C19—C14	120.6 (2)
C3—C4—H4A	109.3	C18—C19—H19	119.7
C3—C4—H4B	109.3	C22—C21—C26	116.83 (19)
H4A—C4—H4B	108.0	C22—C21—N20	119.44 (19)
C5—C4—C3	111.55 (19)	C26—C21—N20	123.7 (2)
C5—C4—H4A	109.3	C23—C22—C21	123.2 (2)
C5—C4—H4B	109.3	F2—C22—C21	117.14 (19)
C4—C5—H5A	109.3	F2—C22—C23	119.6 (2)
C4—C5—H5B	109.3	C22—C23—H23	120.6
C4—C5—C6	111.43 (17)	C22—C23—C24	118.9 (2)
H5A—C5—H5B	108.0	C24—C23—H23	120.6
C6—C5—H5A	109.3	C23—C24—H24	120.2
C6—C5—H5B	109.3	C23—C24—C25	119.7 (2)
C1—C6—C5	112.79 (17)	C25—C24—H24	120.2
C1—C6—H6A	109.0	C24—C25—H25	119.6
C1—C6—H6B	109.0	C24—C25—C26	120.9 (2)
C5—C6—H6A	109.0	C26—C25—H25	119.6
C5—C6—H6B	109.0	C21—C26—H26	119.7
H6A—C6—H6B	107.8	C25—C26—C21	120.5 (2)
C10—C9—H9	109.4	C25—C26—H26	119.7
N13—C9—H9	109.4	C9—N13—H13	118.8 (16)
N13—C9—C10	109.05 (16)	C14—N13—C9	122.94 (17)
N13—C9—O8	106.80 (15)	C14—N13—H13	117.8 (16)
O8—C9—H9	109.4	C10—N20—H20	119.7 (17)
O8—C9—C10	112.70 (15)	C21—N20—C10	122.63 (18)
C9—C10—H10	109.5	C21—N20—H20	117.2 (18)
N20—C10—C9	109.41 (16)	C1—O7—O8	107.68 (12)
N20—C10—H10	109.5	C9—O8—O7	105.55 (12)
N20—C10—O11	105.69 (15)	C10—O11—O12	106.16 (12)
O11—C10—C9	113.15 (15)	C1—O12—O11	107.55 (12)

C1—C2—C3—C4	55.8 (2)	C22—C23—C24—C25	0.3 (4)
C1—O7—O8—C9	106.24 (15)	C23—C24—C25—C26	-0.2 (4)
C2—C1—C6—C5	52.9 (2)	C24—C25—C26—C21	-0.8 (4)
C2—C1—O7—O8	-167.85 (13)	C26—C21—C22—C23	-1.4 (3)
C2—C1—O12—O11	67.08 (18)	C26—C21—C22—F2	178.16 (18)
C2—C3—C4—C5	-56.0 (3)	C26—C21—N20—C10	22.5 (3)
C3—C4—C5—C6	53.4 (3)	F1—C15—C16—C17	-179.4 (2)
C4—C5—C6—C1	-52.1 (3)	F2—C22—C23—C24	-179.1 (2)
C6—C1—C2—C3	-54.1 (2)	N13—C9—C10—N20	-79.4 (2)
C6—C1—O7—O8	70.13 (17)	N13—C9—C10—O11	163.05 (15)
C6—C1—O12—O11	-169.87 (13)	N13—C9—O8—O7	169.53 (13)
C9—C10—N20—C21	150.74 (18)	N13—C14—C15—C16	178.3 (2)
C9—C10—O11—O12	-69.08 (17)	N13—C14—C15—F1	-2.1 (3)
C10—C9—N13—C14	158.18 (18)	N13—C14—C19—C18	-178.02 (19)
C10—C9—O8—O7	-70.73 (17)	N20—C10—O11—O12	171.22 (13)
C10—O11—O12—C1	105.64 (15)	N20—C21—C22—C23	178.7 (2)
C14—C15—C16—C17	0.1 (4)	N20—C21—C22—F2	-1.8 (3)
C15—C14—C19—C18	1.2 (3)	N20—C21—C26—C25	-178.56 (19)
C15—C14—N13—C9	-161.48 (19)	O7—C1—C2—C3	-176.11 (16)
C15—C16—C17—C18	0.4 (4)	O7—C1—C6—C5	170.77 (16)
C16—C17—C18—C19	-0.2 (4)	O7—C1—O12—O11	-48.95 (16)
C17—C18—C19—C14	-0.7 (4)	O8—C9—C10—N20	162.18 (15)
C19—C14—C15—C16	-0.9 (3)	O8—C9—C10—O11	44.6 (2)
C19—C14—C15—F1	178.67 (18)	O8—C9—N13—C14	-79.8 (2)
C19—C14—N13—C9	17.7 (3)	O11—C10—N20—C21	-87.1 (2)
C21—C22—C23—C24	0.5 (4)	O12—C1—C2—C3	65.5 (2)

C22—C21—C26—C25	1.5 (3)	O12—C1—C6—C5	-70.4 (2)
C22—C21—N20—C10	-157.62 (19)	O12—C1—O7—O8	-47.03 (17)

(compound_III)

Crystal data

$C_{20}H_{22}F_2N_2O_4$	$F(000) = 824$
$M_r = 392.40$	$D_x = 1.402$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 12.9687$ (13) Å	Cell parameters from 2159 reflections
$b = 10.0294$ (8) Å	$\theta = 2.0$–$28.7°$
$c = 14.5182$ (15) Å	$\mu = 0.11$ mm^{-1}
$\beta = 100.068$ (9)°	$T = 293$ K
$V = 1859.3$ (3) Å^3	Plank, yellow
$Z = 4$	0.77 × 0.34 × 0.16 mm

Data collection

Xcalibur, Eos diffractometer	4320 independent reflections
Radiation source: Enhance (Mo) X-ray Source	2239 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.051$
Detector resolution: 16.1709 pixels mm^{-1}	$\theta_{max} = 29.1°$, $\theta_{min} = 2.3°$
ω scans	$h = -15 \rightarrow 16$
Absorption correction: multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.37.35 (release 13-08-2014 CrysAlis171 .NET) (compiled Aug 13 2014,18:06:01) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	$k = -13 \rightarrow 12$
$T_{min} = 0.332$, $T_{max} = 1.000$	$l = -18 \rightarrow 12$
9582 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.085$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.235$	$w = 1/[\sigma^2(F_o^2) + (0.084P)^2 + 1.124P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
4320 reflections	$\Delta\rangle_{max}$ = 0.67 e Å^{-3}
261 parameters	$\Delta\rangle_{min}$ = -0.31 e Å^{-3}
0 restraints	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for (compound_III)

	x	y	z	U_{iso}*/U_{eq}
C1	0.8811 (2)	0.5942 (3)	0.5931 (2)	0.0368 (8)
C2	0.8719 (3)	0.6959 (4)	0.5145 (3)	0.0533 (10)
H2A	0.913404	0.666631	0.468759	0.064*
H2B	0.799494	0.701709	0.483506	0.064*
C3	0.9090 (3)	0.8318 (4)	0.5507 (3)	0.0610 (11)
H3A	0.861890	0.866304	0.590044	0.073*
H3B	0.907587	0.892438	0.498452	0.073*
C4	1.0190 (3)	0.8255 (4)	0.6065 (3)	0.0655 (12)
H4A	1.066814	0.796839	0.565949	0.079*
H4B	1.040186	0.913734	0.629716	0.079*
C5	1.0257 (3)	0.7304 (4)	0.6877 (3)	0.0571 (11)
H5A	0.982144	0.762195	0.730974	0.069*
H5B	1.097433	0.725615	0.720736	0.069*
C6	0.9892 (3)	0.5921 (4)	0.6519 (3)	0.0467 (9)
H6A	1.038300	0.556458	0.614973	0.056*
H6B	0.989011	0.533145	0.704873	0.056*
C9	0.7210 (3)	0.3561 (3)	0.5997 (3)	0.0434 (9)
H9	0.692247	0.356739	0.532622	0.052*
C10	0.6734 (3)	0.4718 (3)	0.6459 (2)	0.0377 (8)
H10	0.694274	0.466935	0.714056	0.045*
C14	0.6771 (3)	0.1182 (4)	0.5797 (3)	0.0471 (9)
C15	0.6325 (3)	0.0115 (4)	0.6155 (3)	0.0528 (10)
H15	0.620186	0.014510	0.676676	0.063*
C16	0.6058 (3)	-0.0992 (4)	0.5628 (3)	0.0565 (10)

H16	0.575579	-0.171836	0.587808	0.068*
C17	0.6233 (3)	-0.1030 (4)	0.4747 (3)	0.0547 (10)
C18	0.6689 (4)	-0.0038 (4)	0.4350 (3)	0.0630 (12)
H18	0.681166	-0.011008	0.373917	0.076*
C19	0.6978 (3)	0.1119 (4)	0.4882 (3)	0.0590 (11)
H19	0.730044	0.182798	0.463195	0.071*
C21	0.4950 (3)	0.5408 (3)	0.6671 (2)	0.0363 (8)
C22	0.3884 (3)	0.5175 (4)	0.6439 (3)	0.0437 (9)
H22	0.363878	0.453892	0.598747	0.052*
C23	0.3188 (3)	0.5861 (4)	0.6862 (3)	0.0519 (10)
H23	0.247271	0.570444	0.669993	0.062*
C24	0.3568 (3)	0.6790 (4)	0.7531 (3)	0.0538 (10)
C25	0.4615 (3)	0.7034 (4)	0.7791 (3)	0.0503 (10)
H25	0.485472	0.765931	0.825169	0.060*
C26	0.5308 (3)	0.6337 (4)	0.7358 (3)	0.0451 (9)
H26	0.602290	0.649131	0.752792	0.054*
F1	0.5926 (2)	-0.2147 (2)	0.4222 (2)	0.0916 (10)
F2	0.28814 (19)	0.7512 (3)	0.7942 (2)	0.0919 (10)
N13	0.7003 (3)	0.2335 (3)	0.6360 (2)	0.0528 (9)
H13	0.684 (7)	0.230 (8)	0.706 (7)	0.21 (4)*
N20	0.5636 (2)	0.4684 (3)	0.6213 (2)	0.0476 (8)
H20	0.538 (4)	0.419 (4)	0.581 (3)	0.069 (15)*
O7	0.8529 (2)	0.4717 (2)	0.54477 (18)	0.0484 (7)
O8	0.83419 (18)	0.3693 (2)	0.61166 (19)	0.0496 (7)
O11	0.70413 (16)	0.5990 (2)	0.61189 (16)	0.0391 (6)
O12	0.81273 (17)	0.6203 (2)	0.65769 (15)	0.0386 (6)

Atomic displacement parameters (Å²) for (compound_III)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0317 (17)	0.0376 (19)	0.0428 (19)	-0.0013 (14)	0.0109 (13)	-0.0067 (15)
C2	0.054 (2)	0.061 (3)	0.046 (2)	-0.002 (2)	0.0129 (17)	0.0042 (18)
C3	0.060 (3)	0.049 (2)	0.076 (3)	-0.007 (2)	0.016 (2)	0.015 (2)
C4	0.056 (3)	0.050 (3)	0.095 (3)	-0.020 (2)	0.027 (2)	-0.012 (2)
C5	0.032 (2)	0.065 (3)	0.073 (3)	-0.0088 (18)	0.0043 (18)	-0.016 (2)
C6	0.0334 (19)	0.051 (2)	0.056 (2)	0.0017 (16)	0.0073 (15)	-0.0004 (17)
C9	0.0379 (19)	0.0309 (19)	0.062 (2)	0.0020 (15)	0.0095 (16)	0.0000 (16)
C10	0.0324 (18)	0.0368 (19)	0.0442 (19)	-0.0015 (14)	0.0072 (14)	-0.0013 (15)
C14	0.037 (2)	0.044 (2)	0.060 (2)	0.0050 (17)	0.0062 (16)	-0.0159 (18)
C15	0.051 (2)	0.055 (3)	0.051 (2)	0.0030 (19)	0.0035 (17)	0.0009 (19)

C16	0.052 (2)	0.039 (2)	0.073 (3)	0.0025 (18)	-0.0029 (19)	0.003 (2)
C17	0.055 (2)	0.033 (2)	0.071 (3)	0.0036 (18)	-0.0033 (19)	-0.0175 (19)
C18	0.081 (3)	0.056 (3)	0.055 (3)	0.011 (2)	0.018 (2)	-0.009 (2)
C19	0.065 (3)	0.043 (2)	0.074 (3)	0.000 (2)	0.026 (2)	-0.004 (2)
C21	0.0311 (17)	0.0340 (18)	0.0440 (19)	-0.0026 (14)	0.0076 (14)	-0.0033 (14)
C22	0.0349 (19)	0.041 (2)	0.052 (2)	-0.0017 (16)	-0.0015 (15)	-0.0116 (16)
C23	0.0281 (18)	0.063 (3)	0.062 (2)	0.0001 (17)	-0.0003 (16)	-0.014 (2)
C24	0.036 (2)	0.069 (3)	0.057 (2)	0.0047 (19)	0.0108 (17)	-0.018 (2)
C25	0.041 (2)	0.056 (2)	0.053 (2)	-0.0088 (18)	0.0087 (16)	-0.0213 (18)
C26	0.0328 (18)	0.049 (2)	0.053 (2)	-0.0098 (16)	0.0077 (15)	-0.0120 (17)
F1	0.107 (2)	0.0477 (15)	0.110 (2)	-0.0037 (14)	-0.0087 (18)	-0.0347 (15)
F2	0.0452 (15)	0.129 (2)	0.101 (2)	0.0173 (15)	0.0118 (14)	-0.0599 (19)
N13	0.065 (2)	0.0421 (19)	0.051 (2)	-0.0045 (16)	0.0102 (16)	-0.0032 (15)
N20	0.0285 (15)	0.052 (2)	0.061 (2)	-0.0027 (14)	0.0046 (14)	-0.0205 (17)
O7	0.0510 (16)	0.0443 (15)	0.0534 (16)	-0.0061 (12)	0.0188 (12)	-0.0132 (12)
O8	0.0374 (14)	0.0366 (14)	0.0751 (19)	0.0028 (11)	0.0111 (12)	-0.0010 (12)
O11	0.0274 (12)	0.0362 (13)	0.0520 (15)	0.0027 (10)	0.0021 (10)	0.0009 (10)
O12	0.0327 (12)	0.0413 (14)	0.0420 (13)	-0.0062 (10)	0.0071 (9)	-0.0078 (10)

Geometric parameters (Å, º) for (compound_III)

C1—C2	1.519 (5)	C14—N13	1.417 (5)
C1—C6	1.508 (5)	C15—H15	0.9300
C1—O7	1.431 (4)	C15—C16	1.359 (5)
C1—O12	1.423 (4)	C16—H16	0.9300
C2—H2A	0.9700	C16—C17	1.339 (6)
C2—H2B	0.9700	C17—C18	1.339 (6)
C2—C3	1.509 (6)	C17—F1	1.374 (4)
C3—H3A	0.9700	C18—H18	0.9300
C3—H3B	0.9700	C18—C19	1.408 (6)
C3—C4	1.513 (6)	C19—H19	0.9300
C4—H4A	0.9700	C21—C22	1.384 (5)
C4—H4B	0.9700	C21—C26	1.385 (5)
C4—C5	1.507 (6)	C21—N20	1.402 (4)
C5—H5A	0.9700	C22—H22	0.9300
C5—H5B	0.9700	C22—C23	1.363 (5)
C5—C6	1.527 (5)	C23—H23	0.9300
C6—H6A	0.9700	C23—C24	1.374 (5)
C6—H6B	0.9700	C24—C25	1.367 (5)
C9—H9	0.9800	C24—F2	1.363 (4)

C9—C10	1.525 (5)	C25—H25	0.9300
C9—N13	1.382 (5)	C25—C26	1.373 (5)
C9—O8	1.454 (4)	C26—H26	0.9300
C10—H10	0.9800	N13—H13	1.08 (10)
C10—N20	1.407 (4)	N20—H20	0.79 (5)
C10—O11	1.449 (4)	O7—O8	1.462 (3)
C14—C15	1.362 (5)	O11—O12	1.464 (3)
C14—C19	1.402 (5)		
C6—C1—C2	112.2 (3)	O11—C10—H10	110.1
O7—C1—C2	103.2 (3)	C15—C14—C19	119.4 (4)
O7—C1—C6	113.5 (3)	C15—C14—N13	118.8 (4)
O12—C1—C2	113.3 (3)	C19—C14—N13	121.8 (4)
O12—C1—C6	104.7 (3)	C14—C15—H15	119.6
O12—C1—O7	110.2 (2)	C16—C15—C14	120.7 (4)
C1—C2—H2A	109.3	C16—C15—H15	119.6
C1—C2—H2B	109.3	C15—C16—H16	120.3
H2A—C2—H2B	108.0	C17—C16—C15	119.5 (4)
C3—C2—C1	111.5 (3)	C17—C16—H16	120.3
C3—C2—H2A	109.3	C16—C17—C18	123.5 (4)
C3—C2—H2B	109.3	C16—C17—F1	118.2 (4)
C2—C3—H3A	109.4	C18—C17—F1	118.3 (4)
C2—C3—H3B	109.4	C17—C18—H18	121.0
C2—C3—C4	111.2 (3)	C17—C18—C19	118.1 (4)
H3A—C3—H3B	108.0	C19—C18—H18	121.0
C4—C3—H3A	109.4	C14—C19—C18	118.7 (4)
C4—C3—H3B	109.4	C14—C19—H19	120.6
C3—C4—H4A	109.3	C18—C19—H19	120.6
C3—C4—H4B	109.3	C22—C21—C26	118.9 (3)
H4A—C4—H4B	108.0	C22—C21—N20	119.1 (3)
C5—C4—C3	111.4 (3)	C26—C21—N20	121.9 (3)
C5—C4—H4A	109.3	C21—C22—H22	119.4
C5—C4—H4B	109.3	C23—C22—C21	121.1 (3)
C4—C5—H5A	109.7	C23—C22—H22	119.4
C4—C5—H5B	109.7	C22—C23—H23	120.7
C4—C5—C6	109.7 (3)	C22—C23—C24	118.5 (3)
H5A—C5—H5B	108.2	C24—C23—H23	120.7
C6—C5—H5A	109.7	C25—C24—C23	122.1 (3)
C6—C5—H5B	109.7	F2—C24—C23	119.3 (3)

C1—C6—C5	112.5 (3)	F2—C24—C25	118.6 (3)
C1—C6—H6A	109.1	C24—C25—H25	120.6
C1—C6—H6B	109.1	C24—C25—C26	118.7 (3)
C5—C6—H6A	109.1	C26—C25—H25	120.6
C5—C6—H6B	109.1	C21—C26—H26	119.7
H6A—C6—H6B	107.8	C25—C26—C21	120.5 (3)
C10—C9—H9	108.6	C25—C26—H26	119.7
N13—C9—H9	108.6	C9—N13—C14	122.8 (4)
N13—C9—C10	112.9 (3)	C9—N13—H13	118 (4)
N13—C9—O8	107.2 (3)	C14—N13—H13	118 (4)
O8—C9—H9	108.6	C10—N20—H20	119 (3)
O8—C9—C10	110.9 (3)	C21—N20—C10	124.4 (3)
C9—C10—H10	110.1	C21—N20—H20	117 (3)
N20—C10—C9	109.9 (3)	C1—O7—O8	109.6 (2)
N20—C10—H10	110.1	C9—O8—O7	105.4 (2)
N20—C10—O11	105.2 (3)	C10—O11—O12	105.9 (2)
O11—C10—C9	111.3 (3)	C1—O12—O11	109.6 (2)
C1—C2—C3—C4	54.4 (4)	C22—C21—N20—C10	-172.4 (3)
C1—O7—O8—C9	103.7 (3)	C22—C23—C24—C25	-0.6 (7)
C2—C1—C6—C5	52.6 (4)	C22—C23—C24—F2	178.1 (4)
C2—C1—O7—O8	-166.8 (2)	C23—C24—C25—C26	0.8 (7)
C2—C1—O12—O11	68.4 (3)	C24—C25—C26—C21	0.1 (6)
C2—C3—C4—C5	-58.0 (5)	C26—C21—C22—C23	1.3 (6)
C3—C4—C5—C6	57.2 (4)	C26—C21—N20—C10	6.7 (6)
C4—C5—C6—C1	-54.8 (4)	F1—C17—C18—C19	178.4 (4)
C6—C1—C2—C3	-52.0 (4)	F2—C24—C25—C26	-178.0 (4)
C6—C1—O7—O8	71.5 (3)	N13—C9—C10—N20	-68.8 (4)
C6—C1—O12—O11	-169.0 (2)	N13—C9—C10—O11	175.1 (3)
C9—C10—N20—C21	165.2 (3)	N13—C9—O8—O7	159.9 (3)
C9—C10—O11—O12	-75.8 (3)	N13—C14—C15—C16	177.8 (4)
C10—C9—N13—C14	141.1 (3)	N13—C14—C19—C18	-177.5 (4)
C10—C9—O8—O7	-76.5 (3)	N20—C10—O11—O12	165.3 (2)

C10—O11—O12—C1	103.5 (3)	N20—C21—C22—C23	-179.6 (4)
C14—C15—C16—C17	-0.2 (6)	N20—C21—C26—C25	179.8 (4)
C15—C14—C19—C18	1.8 (6)	O7—C1—C2—C3	-174.5 (3)
C15—C14—N13—C9	-163.7 (4)	O7—C1—C6—C5	169.1 (3)
C15—C16—C17—C18	1.8 (6)	O7—C1—O12—O11	-46.7 (3)
C15—C16—C17—F1	-178.0 (4)	O8—C9—C10—N20	170.9 (3)
C16—C17—C18—C19	-1.5 (7)	O8—C9—C10—O11	54.8 (4)
C17—C18—C19—C14	-0.4 (6)	O8—C9—N13—C14	-96.6 (4)
C19—C14—C15—C16	-1.5 (6)	O11—C10—N20—C21	-74.9 (4)
C19—C14—N13—C9	15.6 (6)	O12—C1—C2—C3	66.3 (4)
C21—C22—C23—C24	-0.4 (6)	O12—C1—C6—C5	-70.7 (4)
C22—C21—C26—C25	-1.2 (6)	O12—C1—O7—O8	-45.5 (3)

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