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Dimethyl (7-hydroxy-4-methyl-2-oxo-2*H*-chromen-3-yl)phosphonate

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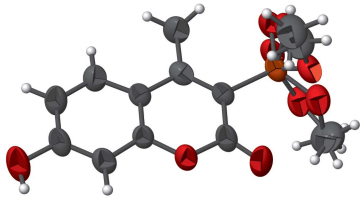
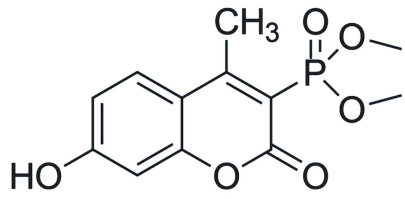
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{12}H_{13}O_6P$, the coumarin ring system is essentially planar [dihedral angle between the rings = 1.32 (16)°] and the methoxy groups and double-bonded O atom of the phosphonate group are disordered over two sets of sites [occupancy ratio 0.537 (2):0.463 (2)]. In the crystal, C—H···O hydrogen bonds involving the disordered phosphonate O atom as acceptor occur, which generate [100] chains. Weak C—H···O and aromatic π–π stacking interactions [minimum centroid–centroid separation = 3.713 (2) Å] are also observed.

3D view



Chemical scheme



Structure description

Several 3-phosphorated coumarins have been proved to exhibit cytotoxicity on some human leukemia cell lines as well as having high alkylating activity (Budzisz *et al.*, 2003) and the selective synthesis of phosphorated coumarins has been a quite active topic (Yuan *et al.*, 2015; Mi *et al.*, 2013). Our group has investigated the phosphorylation of coumarins catalysed by chelating N-heterocyclic palladium complexes and obtained 3-phosphorated coumarins selectively (Yang *et al.*, 2016). The structure of one of these products, *viz*.: the title compound, was characterized unambiguously by single-crystal X-ray diffraction studies.

As shown in Fig. 1, the coumarin ring system is essentially planar [dihedral angle between the rings = 1.32 (16)°]. The methoxyl groups and the double-bonded oxygen atom of the phosphonate group show disorder, with the major and minor components of the disorder having an occupancy factor of 0.537 (2) and 0.463 (2), respectively. In the crystal, O—H···O hydrogen bonds (Table 1) involving the disordered phosphonate group are observed, which generate [100] chains. Weak C—H···O and aromatic π-π stacking interactions [minimum centroid–centroid separation = 3.713 (2) Å] are also observed.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4^{i}	0.82	1.78	2.562 (6)	159
O3—H3···O4A^{i}	0.82	2.01	2.812 (7)	168
C8—H8···O1^{ii}	0.93	2.44	3.220 (4)	142
C10—H10B···O4	0.96	2.22	2.831 (6)	121
C12—H12A···O1	0.96	2.20	2.96 (5)	135

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

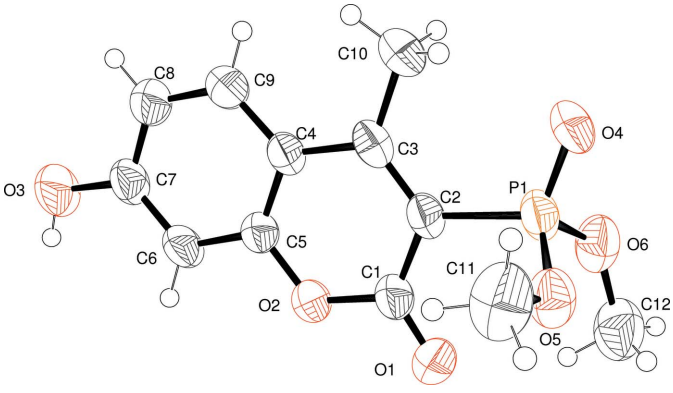


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids. Only the major disorder component is shown.

Synthesis and crystallization

The synthesis of the title compound is based on our reported literature procedure (Yang *et al.*, 2016). A Schlenk tube charged with 7-hydroxy-4-methyl coumarin (0.5 mmol, 88 mg), dimethyl phosphite (1.0 mmol, 110 mg), NHC palladium complex (0.05 mmol), $AgNO_3$ (1.0 mmol, 170 mg) and CH_3CN (2 ml) was heated at 80°C for 10 h. The mixture was then cooled, filtered and the filtrate was evaporated. Purification of the residue by column chromatography (silica, petroleum ether/ethyl acetate = 2/11/4, *v*/*v*) produced the pure products. Recrystallization of the product from CH_2Cl_2/diethyl ether (1/1, *v*/*v*) solution afforded the title compound as colourless prisms.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{13}O_6P$
M_r	284.19
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	9.9684 (7), 7.8695 (6), 16.6927 (10)
β (°)	106.097 (7)
V (Å^3)	1258.13 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.24
Crystal size (mm)	0.25 × 0.12 × 0.1
Data collection	
Diffractometer	Agilent Xcalibur Eos
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.007, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5507, 2572, 1364
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.173, 1.01
No. of reflections	2572
No. of parameters	194
No. of restraints	26
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.28

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

IUCrData (2017). **2**, x171119 [https://doi.org/10.1107/S2414314617011191]

Dimethyl (7-hydroxy-4-methyl-2-oxo-2*H*-chromen-3-yl)phosphonate

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Dimethyl (7-hydroxy-4-methyl-2-oxo-2*H*-chromen-3-yl)phosphonate

Crystal data

$C_{12}H_{13}O_6P$
M_r = 284.19
Monoclinic, $P2_1/c$
a = 9.9684 (7) Å
b = 7.8695 (6) Å
c = 16.6927 (10) Å
β = 106.097 (7)°
V = 1258.13 (16) Å^3
Z = 4
$F(000)$ = 592
D_x = 1.500 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1046 reflections
θ = 3.8–25.4°
μ = 0.24 mm^{-1}
T = 293 K
Prism, colourless
0.25 × 0.12 × 0.1 mm

Data collection

Agilent Xcalibur Eos diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.2312 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku Oxford Diffraction, 2015)
T_{min} = 0.007, T_{max} = 1.000
5507 measured reflections
2572 independent reflections
1364 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 26.4°, θ_{min} = 2.1°
h = −12→11
k = −6→9
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.173
S = 1.01
2572 reflections
194 parameters
26 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0763P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Aromatic H atoms were placed geometrically and refined as riding, with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C). The H atoms associated to hydroxyl and methyl groups were refined as rotating groups, with U_{iso}(H) = 1.5 U_{eq}(C). The O5A—C11A and O6A—C12A bonds were refined with restrained distances of 1.55 (2) Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.4062 (3)	0.3873 (5)	0.6581 (2)	0.0552 (10)	
C2	0.2791 (3)	0.3234 (4)	0.6012 (2)	0.0468 (8)	
C3	0.2797 (3)	0.2579 (5)	0.5251 (2)	0.0486 (9)	
C4	0.4104 (3)	0.2502 (4)	0.5029 (2)	0.0451 (8)	
C5	0.5316 (3)	0.3061 (4)	0.56004 (19)	0.0450 (8)	
C6	0.6615 (3)	0.3005 (5)	0.5456 (2)	0.0547 (10)	
H6	0.7404	0.3383	0.5858	0.066*	
C7	0.6715 (4)	0.2381 (5)	0.4706 (2)	0.0552 (10)	
C8	0.5532 (4)	0.1831 (5)	0.4109 (2)	0.0617 (10)	
H8	0.5604	0.1421	0.3600	0.074*	
C9	0.4261 (4)	0.1891 (5)	0.4269 (2)	0.0562 (10)	
H9	0.3476	0.1516	0.3862	0.067*	
C10	0.1510 (3)	0.1924 (6)	0.4629 (2)	0.0725 (12)	
H10A	0.0967	0.2863	0.4345	0.109*	
H10B	0.0965	0.1275	0.4912	0.109*	
H10C	0.1774	0.1213	0.4230	0.109*	
C11	0.209 (3)	0.077 (3)	0.733 (2)	0.086 (5)	0.537 (2)
H11A	0.1408	0.0093	0.6941	0.129*	0.537 (2)
H11B	0.2170	0.0382	0.7888	0.129*	0.537 (2)
H11C	0.2979	0.0652	0.7215	0.129*	0.537 (2)
C11A	0.209 (4)	0.036 (4)	0.723 (2)	0.086 (5)	0.463 (2)
H11D	0.2358	−0.0589	0.6947	0.129*	0.463 (2)
H11E	0.1707	−0.0036	0.7660	0.129*	0.463 (2)
H11F	0.2893	0.1057	0.7466	0.129*	0.463 (2)
C12	0.151 (5)	0.598 (2)	0.738 (2)	0.085 (3)	0.537 (2)
H12A	0.2501	0.6123	0.7468	0.127*	0.537 (2)
H12B	0.1341	0.5309	0.7816	0.127*	0.537 (2)
H12C	0.1082	0.7076	0.7366	0.127*	0.537 (2)
C12A	0.153 (6)	0.609 (3)	0.727 (3)	0.085 (3)	0.463 (2)
H12D	0.1767	0.6525	0.6793	0.127*	0.463 (2)
H12E	0.2202	0.6479	0.7770	0.127*	0.463 (2)
H12F	0.0618	0.6493	0.7272	0.127*	0.463 (2)
O1	0.4182 (3)	0.4547 (4)	0.72427 (15)	0.0756 (9)	
O2	0.5290 (2)	0.3705 (3)	0.63588 (13)	0.0581 (7)	
O3	0.7946 (3)	0.2292 (4)	0.45079 (16)	0.0806 (9)	
H3	0.8580	0.2619	0.4905	0.121*	
O4	0.0015 (5)	0.2510 (8)	0.5818 (3)	0.0693 (13)	0.537 (2)
O4A	0.0032 (6)	0.3910 (9)	0.5761 (4)	0.0693 (13)	0.463 (2)
O5	0.1688 (5)	0.2446 (7)	0.7256 (3)	0.0615 (10)	0.537 (2)
O5A	0.1013 (5)	0.1394 (7)	0.6613 (3)	0.0615 (10)	0.463 (2)
O6	0.0938 (5)	0.5143 (6)	0.6592 (3)	0.0679 (11)	0.537 (2)
O6A	0.1527 (6)	0.4150 (8)	0.7252 (3)	0.0679 (11)	0.463 (2)
P1	0.12560 (9)	0.32787 (13)	0.63845 (6)	0.0535 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0398 (19)	0.077 (3)	0.052 (2)	0.0053 (19)	0.0172 (17)	0.003 (2)
C2	0.0335 (16)	0.054 (2)	0.0544 (19)	0.0022 (16)	0.0142 (15)	0.0028 (18)
C3	0.0357 (18)	0.050 (2)	0.059 (2)	0.0072 (16)	0.0105 (16)	0.0102 (18)
C4	0.0351 (17)	0.051 (2)	0.0491 (19)	0.0040 (16)	0.0114 (15)	0.0039 (16)
C5	0.0386 (18)	0.052 (2)	0.0452 (18)	0.0016 (16)	0.0134 (15)	0.0002 (16)
C6	0.0325 (17)	0.076 (3)	0.055 (2)	−0.0001 (17)	0.0104 (16)	0.0016 (19)
C7	0.0388 (19)	0.076 (3)	0.054 (2)	0.0070 (19)	0.0188 (17)	0.0088 (19)
C8	0.052 (2)	0.081 (3)	0.055 (2)	0.009 (2)	0.0203 (19)	−0.002 (2)
C9	0.0441 (19)	0.074 (3)	0.0492 (19)	0.0051 (19)	0.0100 (16)	−0.0008 (18)
C10	0.038 (2)	0.106 (4)	0.070 (2)	−0.003 (2)	0.0088 (18)	−0.015 (2)
C11	0.106 (4)	0.060 (11)	0.104 (5)	0.016 (7)	0.048 (5)	0.017 (7)
C11A	0.106 (4)	0.060 (11)	0.104 (5)	0.016 (7)	0.048 (5)	0.017 (7)
C12	0.081 (4)	0.076 (4)	0.102 (8)	0.012 (3)	0.035 (5)	−0.012 (3)
C12A	0.081 (4)	0.076 (4)	0.102 (8)	0.012 (3)	0.035 (5)	−0.012 (3)
O1	0.0553 (15)	0.117 (3)	0.0575 (15)	−0.0005 (16)	0.0202 (13)	−0.0220 (16)
O2	0.0334 (12)	0.088 (2)	0.0542 (14)	−0.0038 (12)	0.0136 (11)	−0.0117 (13)
O3	0.0454 (15)	0.130 (3)	0.0747 (17)	0.0084 (18)	0.0302 (14)	0.0004 (18)
O4	0.0325 (15)	0.106 (4)	0.069 (2)	−0.003 (3)	0.0146 (15)	−0.004 (3)
O4A	0.0325 (15)	0.106 (4)	0.069 (2)	−0.003 (3)	0.0146 (15)	−0.004 (3)
O5	0.059 (2)	0.064 (3)	0.069 (2)	0.0066 (19)	0.030 (2)	0.0139 (18)
O5A	0.059 (2)	0.064 (3)	0.069 (2)	0.0066 (19)	0.030 (2)	0.0139 (18)
O6	0.069 (3)	0.067 (3)	0.076 (3)	0.018 (2)	0.033 (2)	0.008 (2)
O6A	0.069 (3)	0.067 (3)	0.076 (3)	0.018 (2)	0.033 (2)	0.008 (2)
P1	0.0368 (5)	0.0680 (7)	0.0595 (6)	0.0055 (5)	0.0196 (4)	0.0059 (5)

Geometric parameters (Å, º)

C1—C2	1.446 (5)	C11—H11B	0.9600
C1—O1	1.200 (4)	C11—H11C	0.9600
C1—O2	1.381 (4)	C11—O5	1.38 (2)
C2—C3	1.373 (4)	C11A—H11D	0.9600
C2—P1	1.805 (3)	C11A—H11E	0.9600
C3—C4	1.451 (4)	C11A—H11F	0.9600
C3—C10	1.501 (5)	C11A—O5A	1.499 (19)
C4—C5	1.387 (4)	C12—H12A	0.9600
C4—C9	1.405 (4)	C12—H12B	0.9600
C5—C6	1.382 (4)	C12—H12C	0.9600
C5—O2	1.370 (4)	C12—O6	1.43 (4)
C6—H6	0.9300	C12A—H12D	0.9600
C6—C7	1.374 (5)	C12A—H12E	0.9600
C7—C8	1.385 (5)	C12A—H12F	0.9600
C7—O3	1.358 (4)	C12A—O6A	1.529 (19)
C8—H8	0.9300	O3—H3	0.8200
C8—C9	1.366 (4)	O4—P1	1.464 (5)
C9—H9	0.9300	O4A—P1	1.454 (6)

C10—H10A	0.9600	O5—P1	1.543 (4)
C10—H10B	0.9600	O5A—P1	1.567 (5)
C10—H10C	0.9600	O6—P1	1.561 (5)
C11—H11A	0.9600	O6A—P1	1.556 (6)
O1—C1—C2	127.1 (3)	O5—C11—H11C	109.5
O1—C1—O2	114.8 (3)	H11D—C11A—H11E	109.5
O2—C1—C2	118.0 (3)	H11D—C11A—H11F	109.5
C1—C2—P1	116.0 (2)	H11E—C11A—H11F	109.5
C3—C2—C1	120.7 (3)	O5A—C11A—H11D	109.5
C3—C2—P1	123.2 (3)	O5A—C11A—H11E	109.5
C2—C3—C4	119.1 (3)	O5A—C11A—H11F	109.5
C2—C3—C10	123.2 (3)	H12A—C12—H12B	109.5
C4—C3—C10	117.7 (3)	H12A—C12—H12C	109.5
C5—C4—C3	118.9 (3)	H12B—C12—H12C	109.5
C5—C4—C9	115.9 (3)	O6—C12—H12A	109.5
C9—C4—C3	125.2 (3)	O6—C12—H12B	109.5
C6—C5—C4	123.3 (3)	O6—C12—H12C	109.5
O2—C5—C4	121.1 (3)	H12D—C12A—H12E	109.5
O2—C5—C6	115.5 (3)	H12D—C12A—H12F	109.5
C5—C6—H6	120.7	H12E—C12A—H12F	109.5
C7—C6—C5	118.6 (3)	O6A—C12A—H12D	109.5
C7—C6—H6	120.7	O6A—C12A—H12E	109.5
C6—C7—C8	120.3 (3)	O6A—C12A—H12F	109.5
O3—C7—C6	122.6 (3)	C5—O2—C1	121.9 (3)
O3—C7—C8	117.1 (3)	C7—O3—H3	109.5
C7—C8—H8	120.0	C11—O5—P1	119.4 (15)
C9—C8—C7	120.0 (3)	C11A—O5A—P1	123.3 (17)
C9—C8—H8	120.0	C12—O6—P1	125.5 (12)
C4—C9—H9	119.0	C12A—O6A—P1	117.5 (19)
C8—C9—C4	121.9 (3)	O4—P1—C2	114.5 (2)
C8—C9—H9	119.0	O4—P1—O5	113.5 (3)
C3—C10—H10A	109.5	O4—P1—O6	110.2 (3)
C3—C10—H10B	109.5	O4A—P1—C2	112.6 (2)
C3—C10—H10C	109.5	O4A—P1—O5A	110.0 (3)
H10A—C10—H10B	109.5	O4A—P1—O6A	114.2 (3)
H10A—C10—H10C	109.5	O5—P1—C2	105.91 (19)
H10B—C10—H10C	109.5	O5—P1—O6	102.1 (3)
H11A—C11—H11B	109.5	O5A—P1—C2	105.6 (2)
H11A—C11—H11C	109.5	O6—P1—C2	109.8 (2)
H11B—C11—H11C	109.5	O6A—P1—C2	112.6 (2)
O5—C11—H11A	109.5	O6A—P1—O5A	100.9 (3)
O5—C11—H11B	109.5		
C1—C2—C3—C4	1.3 (5)	C7—C8—C9—C4	0.0 (6)
C1—C2—C3—C10	−179.0 (3)	C9—C4—C5—C6	−1.2 (5)
C1—C2—P1—O4	−175.7 (4)	C9—C4—C5—O2	179.1 (3)
C1—C2—P1—O4A	135.4 (4)	C10—C3—C4—C5	−178.5 (3)

C1—C2—P1—O5	−49.9 (4)	C10—C3—C4—C9	1.3 (5)
C1—C2—P1—O5A	−104.6 (3)	C11—O5—P1—C2	−63.3 (18)
C1—C2—P1—O6	59.7 (3)	C11—O5—P1—O4	63.1 (18)
C1—C2—P1—O6A	4.6 (4)	C11—O5—P1—O6	−178.3 (18)
C2—C1—O2—C5	4.3 (5)	C11A—O5A—P1—C2	57 (2)
C2—C3—C4—C5	1.3 (5)	C11A—O5A—P1—O4A	179 (2)
C2—C3—C4—C9	−178.9 (3)	C11A—O5A—P1—O6A	−60 (2)
C3—C2—P1—O4	1.8 (4)	C12—O6—P1—C2	−87 (2)
C3—C2—P1—O4A	−47.0 (4)	C12—O6—P1—O4	146 (2)
C3—C2—P1—O5	127.6 (3)	C12—O6—P1—O5	25 (2)
C3—C2—P1—O5A	73.0 (4)	C12A—O6A—P1—C2	80 (2)
C3—C2—P1—O6	−122.8 (3)	C12A—O6A—P1—O4A	−50 (2)
C3—C2—P1—O6A	−177.9 (3)	C12A—O6A—P1—O5A	−168 (2)
C3—C4—C5—C6	178.6 (3)	O1—C1—C2—C3	176.1 (4)
C3—C4—C5—O2	−1.1 (5)	O1—C1—C2—P1	−6.3 (5)
C3—C4—C9—C8	−178.9 (4)	O1—C1—O2—C5	−175.8 (3)
C4—C5—C6—C7	0.6 (6)	O2—C1—C2—C3	−4.1 (5)
C4—C5—O2—C1	−1.8 (5)	O2—C1—C2—P1	173.5 (2)
C5—C4—C9—C8	0.9 (5)	O2—C5—C6—C7	−179.7 (3)
C5—C6—C7—C8	0.4 (6)	O3—C7—C8—C9	−179.9 (4)
C5—C6—C7—O3	179.5 (3)	P1—C2—C3—C4	−176.1 (2)
C6—C5—O2—C1	178.5 (3)	P1—C2—C3—C10	3.6 (5)
C6—C7—C8—C9	−0.7 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O4^{i}	0.82	1.78	2.562 (6)	159
O3—H3···O4*A*^{i}	0.82	2.01	2.812 (7)	168
C8—H8···O1^{ii}	0.93	2.44	3.220 (4)	142
C10—H10*B*···O4	0.96	2.22	2.831 (6)	121
C12—H12*A*···O1	0.96	2.20	2.96 (5)	135

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, −*y*+1/2, *z*−1/2.