Poly[(4-phenylphosphonato)zinc(II)]

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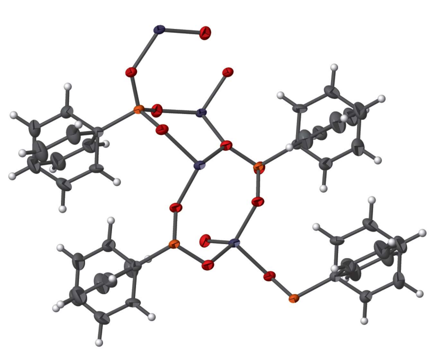
Poly[(μ_4-phenylphosphonato)zinc(II)]

Larry Falvello,[a,b] Paolo Lotti,[a,c] Chiara Massera,[a,d]* Serena C. Tarantino,[a,e] Michele Zema,[a,e] Horst Puschmann,[a,f] Marielle Y. Agbahoungbata,[a] Jacopo Andreo,[a] Suchithra Ashoka Sahadevan,[a] Alessandro Bismuto,[a] Giulia Bonfant,[a] Sourou A. S. Bonou,[a] Claudia Carraro,[a] Marta De Zotti,[a] Armando di Biase,[a] Riccardo Fantini,[a] Ilaria Ferraboschi,[b] Jean Marcos Ferreira Custodio,[a] Matteo Frigerio,[a] Gianpiero Gallo,[a] Silvana Gjyli,[a] Meriem Goudjil,[a] Fernando Igoa,[a] Enver Kahveci,[a] Maksim Kalienko,[a] Sofia Lorenzon,[a] Ludovico Macera,[a] Joaqun Joaqun Manrique Fajardo,[a] Enida Nushi,[a] Said Ouaatta,[a] Emmanuele Parisi,[a] Leonardo Pasqualetto,[a] Edyta Pesko,[a] Giovanni Pierri,[a] Roberta Pinalli,[b] Romy Poppe,[a] Antonio Santoro,[a] Ekaterina Smirnova,[a] Simona Sorbara,[a] Leonardo Tensi[a] and Gers Tusha[a]

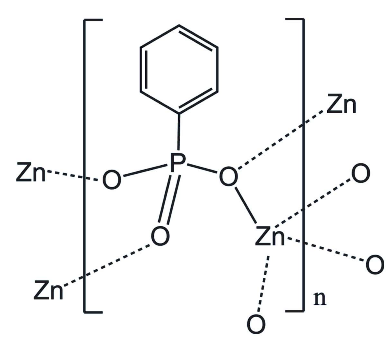
[a]AIC School 2019 – Crystallographic Information Fiesta, Naples, Italy, [b]Department of Inorganic Chemistry, University of Zaragoza, Zaragoza, Spain, [c]Dipartimento di Scienze della Terra, University of Milan, Milan, Italy, [d]Dipartimento di Scienze Chimiche, della Vita e della Sostenibilit Ambientale, University of Parma, Parma, Italy, [e]Dipartimento di Scienze della Terra e dell'Ambiente, University of Pavia, Italy, and [f]OlexSys Ltd, Durham University, Durham, DH1 3LE, UK. *Correspondence e-mail: chiara.massera@unipr.it

The title two-dimensional coordination polymer, $[Zn(C_6H_5PO_3)]_n$, was synthesized serendipitously by reacting a tetraphosphonate cavitand Tiiii[C_3H_7, CH_3, C_6H_5] and $Zn(CH_3COO)_2 \cdot 2H_2O$ in a DMF/H_2O mixture. The basic conditions of the reaction cleaved the phosphonate bridges at the upper rim of the cavitand, making them available for reaction with the zinc ions. The coordination polymer can be described as an inorganic layer in which zinc coordinates the oxygen atoms of the phosphonate groups in a distorted tetrahedral environment, while the phenyl groups, which are statistically disordered over two orientations, point up and down with respect to the layer. The layers interact through van der Waals interactions. The crystal studied was refined as a two-component twin.

3D view



Chemical scheme



Structure description

Resorcinarene-based cavitands (Cram, 1983; Cram & Cram, 1994) are synthetic organic compounds endowed with a rigid, pre-organized cavity which can be decorated both at

Table 1
Selected bond lengths (Å).

Zn1—O1	1.914 (4)	P1—O1	1.507 (4)
Zn1—O2^{i}	1.907 (4)	P1—O2	1.513 (4)
Zn1—O3^{ii}	1.989 (4)	P1—O3	1.561 (4)
Zn1—O3^{iii}	1.988 (4)		

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

the upper and lower rim with different functional groups. In particular, tetraphosphonate cavitands Tiiii have four P═O groups at the upper rim all pointing to the inside of the cavity; they are generally described as Tiiii[R, R_1, R_2], where R = lower rim substituents, R_1 = upper rim substituents and R_2 = substituents on the P atom (Pinalli & Dalcanale, 2013). These dipolar groups can act as hydrogen-bond acceptors and have been used as ligands for metal cations (Pinalli *et al.*, 2016; Melegari *et al.*, 2010). Within the framework of ongoing research on the interactions between cavitands and metal ions, a solvothermal reaction between the tetraphosphonate cavitand Tiiii[C_3H_7, CH_3, C_6H_5] and $Zn(CH_3COO)_2{\cdot}2H_2O$ was carried out in a DMF/H_2O mixture. The basicity of the solution resulting from the presence of the acetate anion hydrolysed the cavitands, cleaving the bridges at the upper rim, with a concomitant release of the phenylphosphonate groups. Their reaction with the zinc cations yielded the title compound, **I**, the crystal structure of which is reported here.

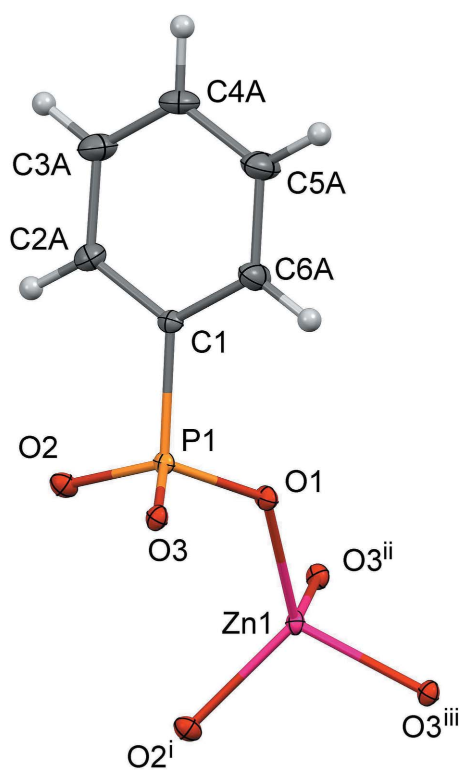


Figure 1
Asymmetric unit of **I**, plus the oxygen atoms needed to complete the tetrahedral coordination around Zn1. Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+1, -y+1, -z+1$. Only one orientation of the disordered phenyl group is shown for clarity.

Table 3
Experimental details.

Crystal data	
Chemical formula	[$Zn(C_6H_5O_3P)$]
M_r	221.47
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	14.8549 (8), 5.1581 (3), 10.5471 (6)
β (°)	105.816 (2)
V (Å^3)	777.56 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.98
Crystal size (mm)	0.10 × 0.08 × 0.07
Data collection	
Diffractometer	Bruker D8 Venture PhotonII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.558, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1897, 1544, 1498
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.121, 1.04
No. of reflections	1544
No. of parameters	138
No. of restraints	144
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.23, −1.08

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *olex2.solve* (Bourhis *et al.*, 2015), *olex2.refine* (Bourhis *et al.*, 2015), *Mercury* (Macrae *et al.*, 2006) and *OLEX2* (Dolomanov *et al.*, 2009).

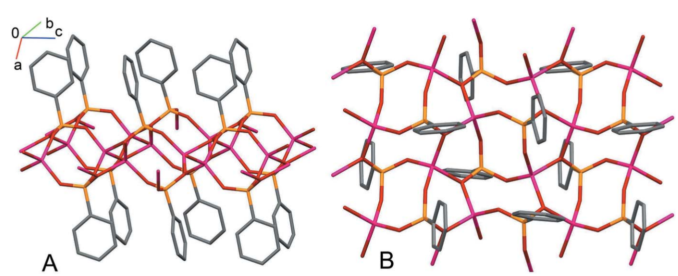


Figure 2
Side (A) and top (B) view of **I** highlighting its layered structure. H atoms have been omitted for clarity.

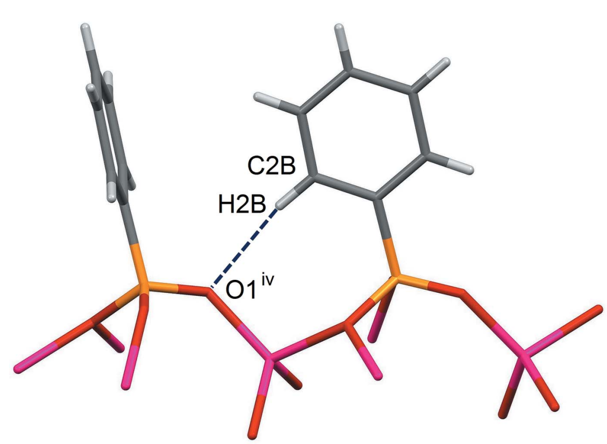


Figure 3
View along the b-axis direction of the intramolecular hydrogen bond (blue dotted line) in **I**. Symmetry code: (iv) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

The asymmetric unit of **I** comprises a phenylphosphonate anion and a zinc(II) cation (Fig. 1); selected bond lengths are given in Table 1. The delocalization of the negative charge and the single/double-bond character within the phosphonate group are shown by the P—O distances, two of which are shorter than the third [P1—O1, P1—O2 and P1—O3 have values of 1.507 (4), 1.513 (4) and 1.561 (4) Å, respectively]. In particular, the longest P—O distance involves the O atom that bridges two metal cations, and it is therefore weakened by the double coordination. The coordination polymer is parallel to the (100) plane; each of the phosphonate groups connects four distinct zinc cations, with O1 and O2 monodentate and with O3 bridging two Zn cations. Overall, the structure can be seen as an inorganic zone, decorated on both sides by the phenyl groups (Fig. 2). Within the layer, the phenyl groups in one orientation form C—H···O hydrogen bonds with the oxygen atoms $O1^{iv}$ of adjacent phosphate groups (see Table 2 and Fig. 3). Cohesion between layers is ensured by dispersion interactions.

A search of the Cambridge Structural Database (Version 5.38, update May 2019; Groom *et al.*, 2016) for phenylphosphonate in combination with zinc, yielded the structure of a *catena*-poly[[aquazinc(II)]-μ_4-phenylphosphonato] (refcode JAHGAA; Martin *et al.*, 1989), closely related to the title compound. The main difference concerns the coordination sphere of the metal ion, which is a distorted octahedron comprising one oxygen atom of a coordinating water molecule and five oxygen atoms from the μ_4-phosphonate groups.

Synthesis and crystallization

The cavitand Tiiii[C_3H_7, CH_3, C_6H_5] was prepared following published procedures (Biavardi *et al.*, 2008): 18.0 mg (0.015 mmol) of the Tiiii cavitand were dissolved in DMF (2 ml), while $Zn(CH_3COO)_2{\cdot}2H_2O$ (6.5 mg, 0.030 mmol) was dissolved in 1 ml of water. The two solutions were put in a Schlenk reactor with a volume of 10 ml, and left at room temperature overnight. The reaction mixture was then heated at 120°C in an oil bath for three days and allowed to cool to room temperature. Small, light-yellow crystals were formed; they were filtered, washed with DMF and dried.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. It was observed that $F_{\rm obs}$ was systematically greater than $F_{\rm calc}$ for the most discrepant reflections. A twin law was identified [−1 0 −0.768 0 −1 0 0 0 1] and for the final refinement, a two-component model was refined. The population of the second component refined to a value of 0.242 (6).

The phenyl ring of the phosphonate group was found to be disordered over two equally populated orientations, related by rotation about the P1—C1···C4 axis. The dihedral angle between the mean planes passing through the two orientations is 76.3 (6)°. Neighbouring disorder assemblies of this type must be populated by alternate disorder groups in order to avoid unreasonably short contacts. That is, for a given orientation of the half-occupied phenyl group, its neighbour must be the other congener. Examination of undistorted reciprocal-lattice plots revealed diffuse streaks, which we interpret as arising from stacking faults accompanying the disorder. We did not undertake more detailed analysis of the diffuse scattering.

Acknowledgements

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full crystallographic data

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Poly[(μ_4-phenylphosphonato)zinc(II)]

Crystal data

[Zn($C_6H_5O_3P$)]	$F(000) = 436.050$
$M_r = 221.47$	$D_x = 1.892$ Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 14.8549$ (8) Å	Cell parameters from 1658 reflections
$b = 5.1581$ (3) Å	$\theta = 6.2$–$74.8°$
$c = 10.5471$ (6) Å	$\mu = 5.98$ mm^{-1}
$\beta = 105.816$ (2)°	$T = 150$ K
$V = 777.56$ (8) Å^3	Prismatic, light yellow
$Z = 4$	0.10 × 0.08 × 0.07 mm

Data collection

Bruker D8 Venture PhotonII diffractometer	1544 independent reflections
phi & ω scan	1498 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2008)	$R_{int} = 0$
$T_{min} = 0.558$, $T_{max} = 0.754$	$\theta_{max} = 72.7°$, $\theta_{min} = 6.2°$
1897 measured reflections	$h = -18 \rightarrow 17$
	$k = -6 \rightarrow 6$
	$l = 0 \rightarrow 12$

Refinement

Refinement on F^2	138 parameters
Least-squares matrix: full	144 restraints
$R[F^2 > 2\sigma(F^2)] = 0.045$	21 constraints
$wR(F^2) = 0.121$	Primary atom site location: iterative
$S = 1.04$	H-atom parameters constrained
1544 reflections	

$w = 1/[\sigma^2(F_o^2) + (0.0246P)^2 + 7.9936P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.0004$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -1.08$ e Å^{-3}

Special details

Refinement. The H atoms bound to C atoms were placed in calculated positions and refined isotropically using a riding model C—H = 0.95 Å, and U_{iso}(H) = 1.2U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.49966 (5)	0.70559 (13)	0.64634 (6)	0.0168 (2)	
P1	0.38324 (9)	0.7695 (3)	0.35527 (12)	0.0175 (3)	
O3	0.4428 (2)	0.6262 (7)	0.2757 (3)	0.0212 (7)	
O2	0.4026 (3)	1.0576 (8)	0.3577 (4)	0.0263 (8)	
O1	0.4016 (2)	0.6435 (8)	0.4888 (3)	0.0233 (8)	
c4	0.0722 (4)	0.6776 (16)	0.1495 (7)	0.0451 (16)	
H4a	0.0075 (4)	0.6593 (16)	0.1062 (7)	0.054 (2)*	0.498 (9)
H4b	0.0074 (4)	0.6583 (16)	0.1066 (7)	0.054 (2)*	0.502 (9)
C1	0.2618 (3)	0.7270 (11)	0.2715 (5)	0.0215 (10)	
C2A	0.2065 (8)	0.945 (3)	0.2247 (12)	0.036 (3)	0.498 (9)
H2A	0.2339 (8)	1.112 (3)	0.2334 (12)	0.043 (3)*	0.498 (9)
C5A	0.1266 (10)	0.459 (3)	0.1968 (17)	0.053 (4)	0.498 (9)
H5A	0.0988 (10)	0.292 (3)	0.1875 (17)	0.063 (4)*	0.498 (9)
C3B	0.1330 (9)	0.725 (3)	0.0761 (13)	0.045 (3)	0.502 (9)
H3B	0.1099 (9)	0.743 (3)	−0.0167 (13)	0.054 (4)*	0.502 (9)
C6B	0.1990 (8)	0.681 (3)	0.3468 (12)	0.037 (3)	0.502 (9)
H6B	0.2215 (8)	0.665 (3)	0.4398 (12)	0.044 (4)*	0.502 (9)
C3A	0.1118 (9)	0.914 (3)	0.1656 (15)	0.050 (4)	0.498 (9)
H3A	0.0741 (9)	1.062 (3)	0.1359 (15)	0.060 (4)*	0.498 (9)
C6A	0.2220 (9)	0.488 (3)	0.2578 (15)	0.041 (3)	0.498 (9)
H6A	0.2593 (9)	0.340 (3)	0.2899 (15)	0.049 (4)*	0.498 (9)
C2B	0.2298 (8)	0.746 (3)	0.1361 (11)	0.034 (3)	0.502 (9)
H2B	0.2722 (8)	0.772 (3)	0.0843 (11)	0.041 (3)*	0.502 (9)
C5B	0.1028 (9)	0.658 (3)	0.2850 (14)	0.047 (3)	0.502 (9)
H5B	0.0597 (9)	0.629 (3)	0.3355 (14)	0.056 (4)*	0.502 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0222 (3)	0.0162 (4)	0.0129 (3)	−0.0007 (3)	0.0061 (3)	0.0004 (2)
P1	0.0189 (6)	0.0221 (6)	0.0123 (5)	−0.0009 (5)	0.0056 (5)	−0.0003 (5)
O3	0.0247 (17)	0.0233 (18)	0.0164 (16)	0.0013 (14)	0.0069 (14)	0.0014 (14)
O2	0.0238 (17)	0.028 (2)	0.029 (2)	−0.0011 (15)	0.0114 (15)	−0.0033 (16)
O1	0.0227 (17)	0.033 (2)	0.0151 (16)	−0.0046 (15)	0.0059 (13)	0.0025 (15)
c4	0.022 (3)	0.059 (4)	0.048 (4)	−0.002 (3)	0.000 (2)	−0.006 (3)
C1	0.020 (2)	0.028 (3)	0.017 (2)	−0.0016 (18)	0.0051 (18)	−0.0021 (19)
C2A	0.031 (5)	0.040 (6)	0.034 (6)	0.003 (3)	0.002 (4)	0.004 (4)
C5A	0.031 (6)	0.050 (7)	0.071 (9)	−0.008 (4)	0.004 (4)	−0.006 (5)

C3B	0.030 (6)	0.069 (9)	0.028 (6)	−0.002 (4)	−0.005 (3)	−0.003 (4)
C6B	0.027 (5)	0.059 (8)	0.026 (5)	−0.004 (4)	0.010 (3)	0.001 (4)
C3A	0.029 (6)	0.060 (8)	0.054 (8)	0.003 (4)	0.000 (4)	−0.001 (4)
C6A	0.030 (6)	0.032 (6)	0.059 (8)	−0.004 (3)	0.008 (4)	−0.003 (4)
C2B	0.032 (5)	0.055 (7)	0.013 (4)	−0.003 (4)	0.003 (3)	0.001 (4)
C5B	0.022 (5)	0.069 (9)	0.048 (6)	−0.004 (4)	0.010 (4)	0.002 (4)

Geometric parameters (Å, º)

Zn1—O1	1.914 (4)	C1—C6A	1.358 (14)
Zn1—O2^{i}	1.907 (4)	C1—C2B	1.380 (12)
Zn1—O3^{ii}	1.989 (4)	C2A—H2A	0.9500
Zn1—O3^{iii}	1.988 (4)	C2A—C3A	1.384 (18)
P1—O1	1.507 (4)	C5A—H5A	0.9500
P1—O2	1.513 (4)	C5A—C6A	1.396 (18)
P1—O3	1.561 (4)	C3B—H3B	0.9500
P1—C1	1.793 (5)	C3B—C2B	1.408 (16)
c4—C5A	1.397 (18)	C6B—H6B	0.9500
c4—C3B	1.362 (16)	C6B—C5B	1.404 (17)
c4—C3A	1.343 (18)	C3A—H3A	0.9500
c4—C5B	1.380 (16)	C6A—H6A	0.9500
C1—C2A	1.398 (14)	C2B—H2B	0.9500
C1—C6B	1.401 (13)	C5B—H5B	0.9500
O2^{i}—Zn1—O3^{iii}	108.46 (16)	C3B—c4—H4b	119.4 (6)
O2^{i}—Zn1—O3^{ii}	101.79 (16)	C3A—c4—H4a	120.1 (7)
O1—Zn1—O3^{iii}	110.74 (16)	C3A—c4—C5A	119.7 (9)
O1—Zn1—O3^{ii}	107.71 (15)	C5B—c4—H4b	119.4 (6)
O1—Zn1—O2^{i}	119.43 (16)	C5B—c4—C3B	121.3 (8)
O2—P1—O3	110.0 (2)	C6A—C1—C2A	119.7 (8)
O1—P1—O3	108.2 (2)	C2B—C1—C6B	120.3 (8)
O1—P1—O2	115.0 (2)	C3A—C2A—H2A	120.2 (9)
C1—P1—O3	108.6 (2)	C6A—C5A—H5A	120.2 (9)
C1—P1—O2	106.8 (2)	C2B—C3B—H3B	119.6 (7)
C1—P1—O1	108.0 (2)	C5B—C6B—H6B	119.9 (8)
P1—O3—Zn1^{iv}	124.8 (2)	H3A—C3A—C2A	119.4 (9)
P1—O3—Zn1^{iii}	115.35 (19)	H6A—C6A—C5A	119.9 (9)
P1—O2—Zn1^{i}	140.5 (2)	H2B—C2B—C3B	120.6 (7)
P1—O1—Zn1	129.8 (2)	H5B—C5B—C6B	120.6 (8)
C5A—c4—H4a	120.1 (7)		
Zn1^{iii}—O3—P1—O2	138.3 (2)	Zn1^{i}—O2—P1—O3	−29.8 (4)
Zn1^{iv}—O3—P1—O2	−19.8 (3)	Zn1^{i}—O2—P1—O1	92.6 (4)
Zn1^{iv}—O3—P1—O1	−146.2 (2)	Zn1^{i}—O2—P1—C1	−147.5 (4)
Zn1^{iii}—O3—P1—O1	12.0 (3)	Zn1—O1—P1—O3	85.0 (3)

$Zn1^{iii}$—O3—P1—C1	−105.1 (3)	Zn1—O1—P1—O2	−38.3 (4)
$Zn1^{iv}$—O3—P1—C1	96.7 (3)	Zn1—O1—P1—C1	−157.5 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2*B*—H2*B*···$O1^{iv}$	0.95	2.45	3.378 (13)	170

Symmetry code: (iv) $x, -y+3/2, z-1/2$.