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Crystal structure of a (carboxymethyl) triethylazanium bromide–2-(triethylazaniumyl) acetate (1/1) hydrogen-bonded dimer

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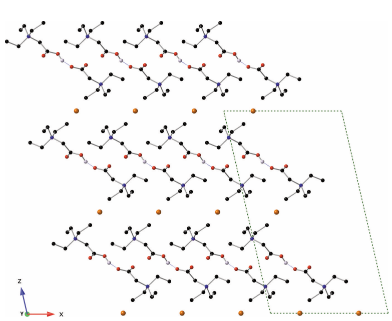
The title compound, $C_8H_{18}NO_2^+ \cdot Br^- \cdot C_8H_{17}NO_2$, crystallizes as the bromide salt of a 50:50 mixture of (triethylazaniumyl)carboxylic acid and the zwitterionic (triethylazaniumyl)carboxylate. The two organic entities are linked by a half-occupied bridging carboxylic acid hydrogen atom that is hydrogen-bonded to the carboxylate group of the second molecule. The tetralkylammonium group adopts a nearly perfect tetrahedral shape around the nitrogen atom with bond lengths that agree with known values. The carboxylic acid/carboxylate group is oriented *anti* to one of the ethyl groups on the ammonium group, and the carbonyl oxygen atom is engaged in intramolecular C—H···O hydrogen bonds.

1. Chemical context

The β-carbonylphosphonate moiety is commonly used as a reagent in the Horner–Wadsworth–Emmons reaction (Horner *et al.*, 1958; Wadsworth & Emmons, 1961; Bisceglia & Orelli, 2015). These molecules are reacted with aldehydes or ketones to prepare α,β-unsaturated esters, where a preference for the *Z*-configuration of the alkene group is often observed. When the phosphonate group is replaced with a phosphine oxide, these sets of compounds have found use as ligands and extraction agents for *f*-elements (Babecki *et al.*, 1989, 1990, 1992). Our research group has also characterized the ability of these types of compounds to sensitize the luminescence of lanthanide ions (Leach *et al.*, 2017; Sartain *et al.*, 2015). To this end, our group has been working to develop a synthetic route to the target compound shown in Fig. 1, following the procedure reported by Ando (1999). The title compound was an undesired byproduct of this reaction, and serendipitously crystallized from the aqueous washings upon standing. A



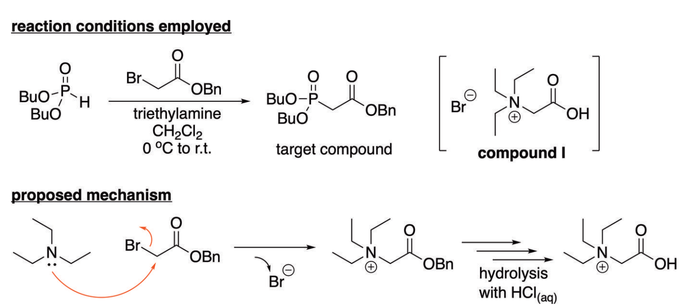


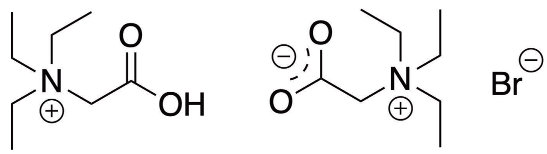
Figure 1
(top) The reaction carried out in this work, along with structures of the target β-carbonylphosphonate and the title compound **I**. (bottom) A proposed mechanism for the formation of the title compound.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.97	1.50	2.457 (4)	167
C3—H3A···O2	0.99	2.39	2.969 (3)	116
C7—H7B···O2	0.99	2.39	3.068 (3)	125

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

proposed mechanism for the formation of the title compound **I** is also shown in Fig. 1.



2. Structural commentary

The title salt crystallizes as a 50:50 mixture of the ammonium carboxylate zwitterion and the ammonium bromide. The molecular entities of this compound are shown in Fig. 2 along with the atom-numbering scheme. The asymmetric unit is composed of all of the atoms shown in Fig. 2 where the carboxylic acid hydrogen atom H1 has a 0.50 occupancy, and the Br^{-} anion is located on a twofold rotation axis (Wyckoff position 4*e*) of space group *I*2/*a*. The ammonium group has C—N bond lengths ranging from 1.514 (3) to 1.526 (3) Å with a nearly perfect tetrahedral arrangement of alkyl groups around the nitrogen atom with a τ_4 descriptor for fourfold coordination of 0.97 (where 0.00 = square-planar, 0.85 = trigonal–pyramidal, and 1.00 = tetrahedral; Yang *et al.*, 2007). The carboxylic acid group has C—O bond lengths of 1.286 (3) and 1.224 (3) Å. When the molecule is viewed down the C2—N1 bond the groups adopt a staggered conformation with the carboxylic acid group being *anti* to the C5–C6 ethyl group. The torsion angle between these two groups (C1—C2—N1—C5) is 168.8 (2)°. Two intramolecular

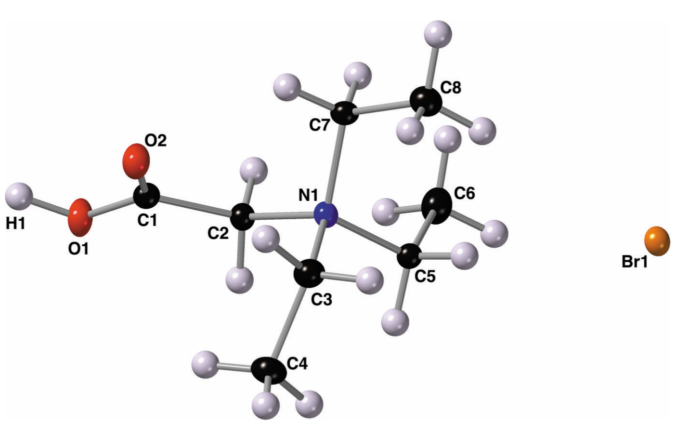


Figure 2
The molecular structure of compound **I**, with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level using standard CPK colors. Atom H1 shows half-occupancy.

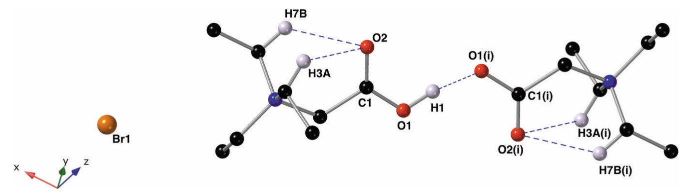


Figure 3
A depiction of the hydrogen-bonding interactions present in the crystal of compound **I** using a ball-and-stick model with standard CPK colors. Hydrogen-bonding interactions are depicted with blue dashed lines and all hydrogen atoms not involved in a hydrogen bond are not shown for clarity.

C—H···O hydrogen bonds are present between the carbonyl oxygen atom O2 and hydrogen atoms H3*A* and H7*B* of the *gauche* alkyl groups (Table 1, Fig. 3).

3. Supramolecular features

Molecules of the title compound exist as hydrogen-bonded dimers in the solid state. The carboxylic acid hydrogen atom H1 is a half-occupied bridging hydrogen atom (Fábry, 2018), and within this dimer it is either bonded to oxygen atom O1 or to its symmetry derived counterpart O1^{i} [symmetry code: (i) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$; Fig. 3]. When this atom H1 is covalently bonded to O1, it is engaged in a very strong asymmetric hydrogen bond with the symmetry-derived oxygen atom O1^{i} (Table 1). The bromide counter-ions are located away from the carboxylate/carboxylic acid sites and occupy a layer that lies parallel to the *ab* plane. These layers are bordered by the ethyl chains of the ammonium groups (Fig. 4).

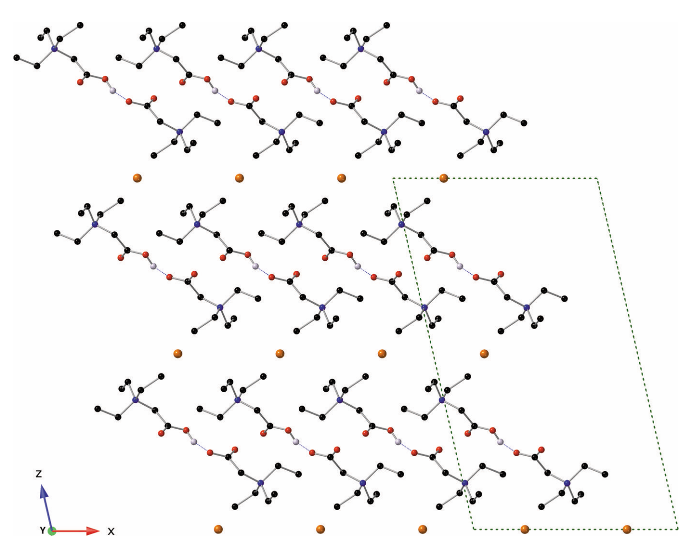


Figure 4
A view of the crystal structure down the *b* axis showing a cross section of the layers of bromide ions. This figure was drawn with a ball-and-stick model using standard CPK colors. Only one position of hydrogen atom H1 is shown, and all other hydrogen atoms have been omitted for clarity.

4. Database survey

A search of the Cambridge Structural Database (CSD version 5.43, Jun. 2022; Groom *et al.*, 2016) for structures with a hydrogen atom shared between two carboxylate sites resulted in 274 hits. One of the simplest structures in this set is that of ammonium diacetate (ACAMAC; Nahringbauer, 1969). The structures ALUNIE (Dega-Szafran *et al.*, 2003) and CIVKUQ (Ghazaryan *et al.*, 2018) are similar to the title compound with either a piperidinium ring or a trimethylammonium group, respectively, in the place of the triethylammonium groups. Both compounds were isolated with a halide counter-ion: ALUNIE was isolated with one chloride anion and CIVKUQ was isolated as the iodide salt.

5. Synthesis and crystallization

Dibutyl phosphite (1.4 ml, 1.4 g, 7.17 mmol) was added *via* syringe to a two-necked 25 ml round-bottom flask under an atmosphere of nitrogen. The reagent was dissolved in 7.0 ml of dichloromethane and the flask was placed in an ice–water bath. Benzyl bromoacetate (1.1 ml, 1.6 g, 6.94 mmol) and triethylamine (1.4 ml, 1.0 g, 10.0 mmol) were added and the reaction mixture was stirred for 15 minutes in the ice bath followed by one hour at room temperature. Water (10 ml) was added to the reaction, and the aqueous layer was washed with ethyl acetate (3×10 ml). The organic extracts were combined and washed with 1 *M* HCl (3×10 ml) and brine (1×10 ml), then dried over $MgSO_4$. The title compound crystallized serendipitously from the combined aqueous washings after standing for *ca* three days.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms bonded to carbon atoms were placed in calculated positions and refined as riding: C—H = 0.95 – 1.00 Å with $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene hydrogen atoms and $U_{iso}(H) = 1.5U_{eq}(C)$ for the hydrogen atoms of the methyl groups. The carboxylic acid hydrogen atom H1 was located using electron-density difference maps. The position of this hydrogen atom was fixed and the occupancy constrained to 0.5. Its isotropic displacement parameter was refined as suggested by Fábry (2018).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_{18}NO_2^+\cdot Br^-\cdot C_8H_{17}NO_2$
M_r	399.37
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	100
a, *b*, *c* (Å)	12.6692 (4), 7.0967 (3), 22.3413 (9)
β (°)	103.022 (4)
V (Å^3)	1957.04 (13)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.03
Crystal size (mm)	0.42 × 0.13 × 0.02
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian (*CrysAlis PRO*; Oxford Diffraction, 2006)
T_{min}, T_{max}	0.568, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6198, 1998, 1785
R_{int}	0.052
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.109, 1.08
No. of reflections	1998
No. of parameters	109
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.89, −0.42

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2006), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *CrystalMaker* (Palmer, 2007), and *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015).

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Crystal structure of a (carboxymethyl)triethylazanium bromide–2-(triethylazaniumyl)acetate (1/1) hydrogen-bonded dimer

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2006); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2006); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *CrystalMaker* (Palmer, 2007); software used to prepare material for publication: Olex2 (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015).

(Carboxymethyl)triethylazanium bromide–2-(triethylazaniumyl)acetate (1/1)

Crystal data

$C_8H_{18}NO_2^+\cdot Br^-\cdot C_8H_{17}NO_2$
$M_r = 399.37$
Monoclinic, $I2/a$
$a = 12.6692$ (4) Å
$b = 7.0967$ (3) Å
$c = 22.3413$ (9) Å
$\beta = 103.022$ (4)°
$V = 1957.04$ (13) Å^3
$Z = 4$
$F(000) = 848$
$D_x = 1.355$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 3269 reflections
$\theta = 6.6$–79.4°
$\mu = 3.03$ mm^{-1}
$T = 100$ K
Plate, colourless
0.42 × 0.13 × 0.02 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Oxford Diffraction, 2006)
$T_{min} = 0.568$, $T_{max} = 1.000$
6198 measured reflections
1998 independent reflections
1785 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 80.0°$, $\theta_{min} = 4.1°$
$h = -11 \rightarrow 16$
$k = -8 \rightarrow 8$
$l = -28 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.109$
$S = 1.08$
1998 reflections
109 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 1.4873P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ 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.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.250000	0.39582 (5)	0.500000	0.01824 (16)	
O1	0.70415 (15)	0.3474 (3)	0.28191 (9)	0.0250 (4)	
H1	0.734798	0.280169	0.252098	0.07 (3)*	0.5
O2	0.57904 (15)	0.1209 (3)	0.27312 (9)	0.0235 (4)	
N1	0.49061 (15)	0.3014 (3)	0.36825 (9)	0.0146 (4)	
C1	0.61984 (19)	0.2698 (4)	0.29428 (11)	0.0181 (5)	
C2	0.57456 (19)	0.3923 (3)	0.33887 (12)	0.0155 (5)	
H2A	0.635817	0.434190	0.372016	0.019*	
H2B	0.542009	0.506334	0.316589	0.019*	
C3	0.5279 (2)	0.1112 (3)	0.39641 (12)	0.0187 (5)	
H3A	0.522278	0.017911	0.362887	0.022*	
H3B	0.477980	0.070888	0.422252	0.022*	
C4	0.6431 (2)	0.1076 (4)	0.43539 (14)	0.0242 (6)	
H4A	0.694224	0.132344	0.409276	0.036*	
H4B	0.658203	−0.016535	0.454658	0.036*	
H4C	0.651144	0.204548	0.467320	0.036*	
C5	0.47364 (19)	0.4306 (4)	0.41955 (11)	0.0168 (5)	
H5A	0.419692	0.371758	0.439611	0.020*	
H5B	0.542724	0.439647	0.450705	0.020*	
C6	0.4358 (2)	0.6278 (4)	0.39983 (14)	0.0255 (6)	
H6A	0.369669	0.621107	0.367223	0.038*	
H6B	0.492434	0.693461	0.384459	0.038*	
H6C	0.420881	0.696650	0.435042	0.038*	
C7	0.38591 (18)	0.2757 (4)	0.31950 (11)	0.0170 (5)	
H7A	0.360683	0.400804	0.302461	0.020*	
H7B	0.401558	0.198822	0.285550	0.020*	
C8	0.2954 (2)	0.1824 (4)	0.34289 (13)	0.0242 (6)	
H8A	0.228952	0.182944	0.310402	0.036*	
H8B	0.283092	0.251692	0.378634	0.036*	
H8C	0.315681	0.052079	0.354755	0.036*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0155 (2)	0.0211 (2)	0.0191 (2)	0.000	0.00614 (14)	0.000
O1	0.0209 (9)	0.0313 (10)	0.0264 (10)	−0.0062 (8)	0.0132 (8)	−0.0083 (8)
O2	0.0214 (9)	0.0270 (10)	0.0242 (10)	−0.0037 (7)	0.0091 (8)	−0.0089 (7)
N1	0.0128 (8)	0.0161 (10)	0.0154 (10)	−0.0009 (7)	0.0043 (8)	0.0001 (8)
C1	0.0161 (10)	0.0229 (13)	0.0149 (12)	0.0010 (9)	0.0029 (9)	−0.0013 (9)

C2	0.0138 (10)	0.0171 (12)	0.0162 (12)	−0.0029 (8)	0.0050 (9)	−0.0002 (9)
C3	0.0212 (12)	0.0158 (12)	0.0186 (12)	0.0001 (8)	0.0035 (10)	0.0024 (9)
C4	0.0213 (12)	0.0252 (14)	0.0233 (14)	0.0057 (10)	−0.0010 (10)	0.0019 (10)
C5	0.0151 (10)	0.0214 (12)	0.0140 (11)	0.0015 (9)	0.0033 (9)	−0.0002 (9)
C6	0.0315 (14)	0.0214 (14)	0.0255 (15)	0.0075 (10)	0.0107 (12)	0.0003 (10)
C7	0.0136 (9)	0.0218 (12)	0.0145 (11)	−0.0025 (9)	0.0008 (9)	−0.0003 (9)
C8	0.0159 (11)	0.0331 (15)	0.0231 (13)	−0.0068 (10)	0.0032 (10)	−0.0005 (11)

Geometric parameters (Å, º)

O1—H1	0.9686	C4—H4B	0.9800
O1—C1	1.286 (3)	C4—H4C	0.9800
O2—C1	1.224 (3)	C5—H5A	0.9900
N1—C2	1.514 (3)	C5—H5B	0.9900
N1—C3	1.519 (3)	C5—C6	1.512 (4)
N1—C5	1.520 (3)	C6—H6A	0.9800
N1—C7	1.526 (3)	C6—H6B	0.9800
C1—C2	1.528 (3)	C6—H6C	0.9800
C2—H2A	0.9900	C7—H7A	0.9900
C2—H2B	0.9900	C7—H7B	0.9900
C3—H3A	0.9900	C7—C8	1.515 (3)
C3—H3B	0.9900	C8—H8A	0.9800
C3—C4	1.522 (4)	C8—H8B	0.9800
C4—H4A	0.9800	C8—H8C	0.9800
C1—O1—H1	114.7	H4A—C4—H4C	109.5
C2—N1—C3	112.00 (18)	H4B—C4—H4C	109.5
C2—N1—C5	107.61 (18)	N1—C5—H5A	108.4
C2—N1—C7	108.91 (18)	N1—C5—H5B	108.4
C3—N1—C5	107.89 (19)	H5A—C5—H5B	107.5
C3—N1—C7	109.20 (19)	C6—C5—N1	115.3 (2)
C5—N1—C7	111.24 (17)	C6—C5—H5A	108.4
O1—C1—C2	110.4 (2)	C6—C5—H5B	108.4
O2—C1—O1	125.8 (2)	C5—C6—H6A	109.5
O2—C1—C2	123.7 (2)	C5—C6—H6B	109.5
N1—C2—C1	116.35 (19)	C5—C6—H6C	109.5
N1—C2—H2A	108.2	H6A—C6—H6B	109.5
N1—C2—H2B	108.2	H6A—C6—H6C	109.5
C1—C2—H2A	108.2	H6B—C6—H6C	109.5
C1—C2—H2B	108.2	N1—C7—H7A	108.7
H2A—C2—H2B	107.4	N1—C7—H7B	108.7
N1—C3—H3A	108.5	H7A—C7—H7B	107.6
N1—C3—H3B	108.5	C8—C7—N1	114.2 (2)
N1—C3—C4	114.9 (2)	C8—C7—H7A	108.7
H3A—C3—H3B	107.5	C8—C7—H7B	108.7
C4—C3—H3A	108.5	C7—C8—H8A	109.5
C4—C3—H3B	108.5	C7—C8—H8B	109.5
C3—C4—H4A	109.5	C7—C8—H8C	109.5

C3—C4—H4B	109.5	H8A—C8—H8B	109.5
C3—C4—H4C	109.5	H8A—C8—H8C	109.5
H4A—C4—H4B	109.5	H8B—C8—H8C	109.5

O1—C1—C2—N1	−167.3 (2)	C3—N1—C7—C8	56.4 (3)
O2—C1—C2—N1	13.8 (4)	C5—N1—C2—C1	168.8 (2)
C2—N1—C3—C4	46.5 (3)	C5—N1—C3—C4	−71.8 (3)
C2—N1—C5—C6	59.1 (3)	C5—N1—C7—C8	−62.6 (3)
C2—N1—C7—C8	179.0 (2)	C7—N1—C2—C1	−70.5 (3)
C3—N1—C2—C1	50.4 (3)	C7—N1—C3—C4	167.2 (2)
C3—N1—C5—C6	−179.9 (2)	C7—N1—C5—C6	−60.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.97	1.50	2.457 (4)	167
C3—H3*A*···O2	0.99	2.39	2.969 (3)	116
C7—H7*B*···O2	0.99	2.39	3.068 (3)	125

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