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Diisopropylammonium 4-methoxybenzoate

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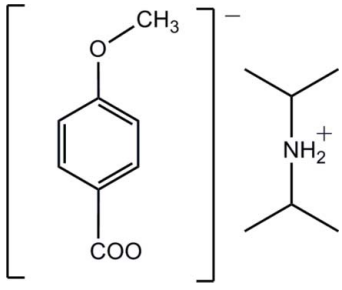
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.058; wR factor = 0.163; data-to-parameter ratio = 20.8.

In the crystal structure of the title compound, $C_6H_{16}N^+\cdot C_8H_7O_3^-$, intermolecular N—H···O hydrogen bonds link the cations and anions into arrangements consisting of two cations and two anions each.

Related literature

For background to organic phase-transition materials, see: Fu *et al.* (2009); Rheinstädter *et al.* (2002); Wu *et al.* (2011).



Experimental

Crystal data

$C_6H_{16}N^+\cdot C_8H_7O_3^-$
M_r = 253.33
Triclinic, $P\overline{1}$
a = 7.3265 (15) Å
b = 8.8808 (18) Å
c = 12.107 (2) Å
α = 87.83 (3)°
β = 77.83 (3)°
γ = 83.44 (3)°
V = 764.9 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.842, T_{max} = 1.000
7992 measured reflections
3501 independent reflections
1945 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.163
S = 1.04
3501 reflections
168 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 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—H1B···O3^{i}	0.90	1.84	2.720 (2)	166
N1—H1A···O2^{ii}	0.90	1.83	2.721 (2)	169

Symmetry codes: (i) $x, y, z-1$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author is grateful to the starter fund of Southeast University for the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2287).

References

Fu, D.-W., Ge, J.-Z., Dai, J., Ye, H.-Y. & Qu, Z.-R. (2009). *Inorg. Chem. Commun.* **12**, 994–997.
Rheinstädter, M. C., Kityk, A. V., Klöpperpieper, A. & Knorr, K. (2002). *Phys. Rev. B*, **66**, 064105.
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Wu, D.-H., Ge, J.-Z., Cai, H.-L., Weng, Z. & Xiong, R.-G. (2011). *CrystEngComm*, **13**, 319–324.

supporting information

Acta Cryst. (2011). E**67**, o1865 [doi:10.1107/S1600536811023762]

Diisopropylammonium 4-methoxybenzoate

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S1. Comment

One of our main research topics is the search for new dielectric-ferroelectric materials. Recent studies have revealed that organic salts might also have this kind of character (Fu *et al.*, 2009; Rheinstädter *et al.*, 2002; Wu *et al.*, 2011). The dielectric constant of the title compound, diisopropylammonium 4-methoxy-benzoate, as a function of temperature indicates that the permittivity is basically temperature-independent. Below the melting point (438–440 K) of the title compound, we have found no dielectric disuniform from 80 K to 405 K. Herein we describe the crystal structure of this compound.

The asymmetric unit of the title compound consists of a diisopropylammonium cation and a 4-methoxybenzoate anion (Fig. 1). Intermolecular N—H···O hydrogen bonds (N1–H1A···O2 1.832 (2) Å, N1–H1B···O3 1.838 (2) Å) link the cations and anions into planar arrangements of two cations and anions each (Fig. 2 and Tab. 1).

S2. Experimental

The title compound was obtained by the addition of *para*-methoxybenzoic acid (1.52 g, 0.01 mol) to a solution of diisopropylamine (1.02 g, 0.01 mol) in methanol in a 1: 1 ratio. Good quality single crystals were obtained by slow evaporation of the solvent after two days (yield: 37%).

S3. Refinement

Positional parameters of all the H atoms bonded to C atom were calculated geometrically with C—H = 0.93 Å (CH_{ar}), 0.98 Å (CH), 0.96 Å (CH_3), with U_{iso}(H) = 1.2 U_{eq}(CH_{ar}, CH) and U_{iso}(H) = 1.5 U_{eq}(CH_3). Nitrogen bound H atoms were locatd in a difference Fourier map and refined freely

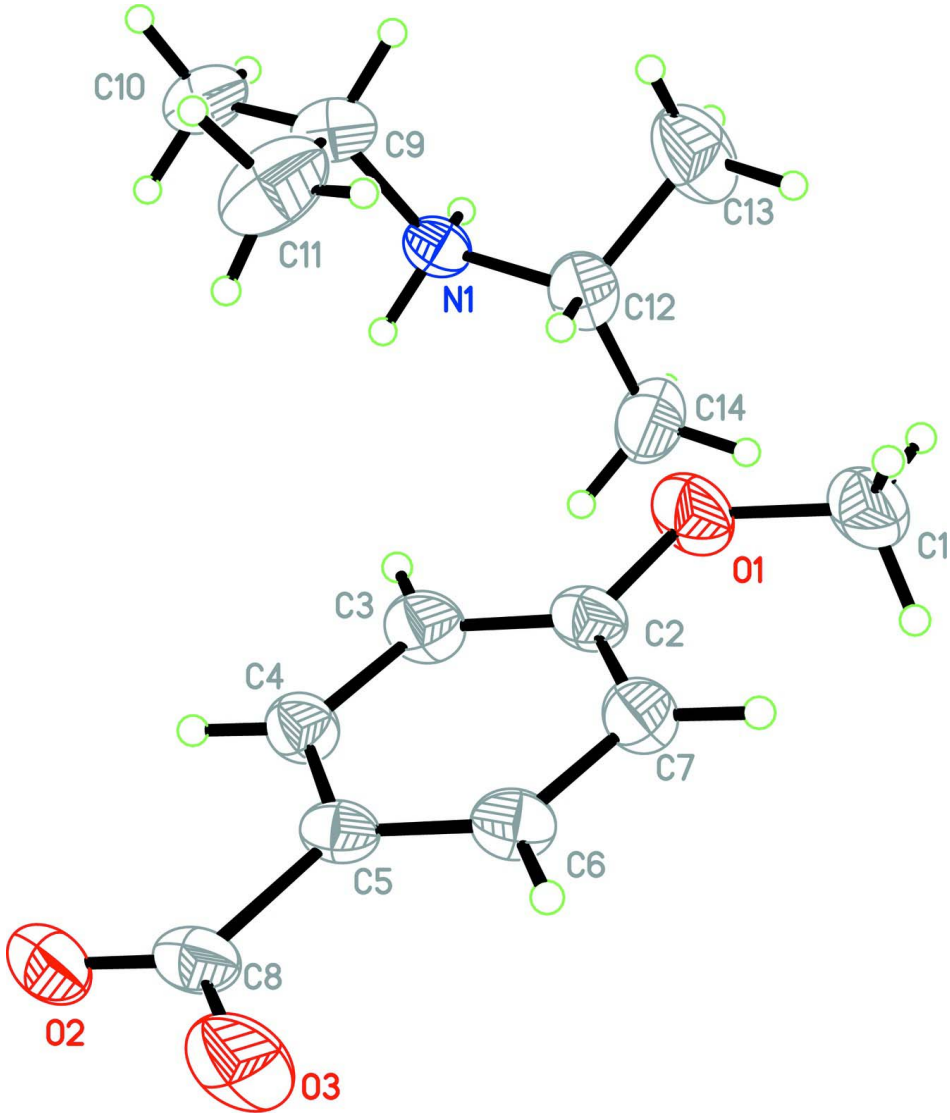

Figure 1

Molecular structure of the title compound, displacement ellipsoids are drawn at the 30% probability level.

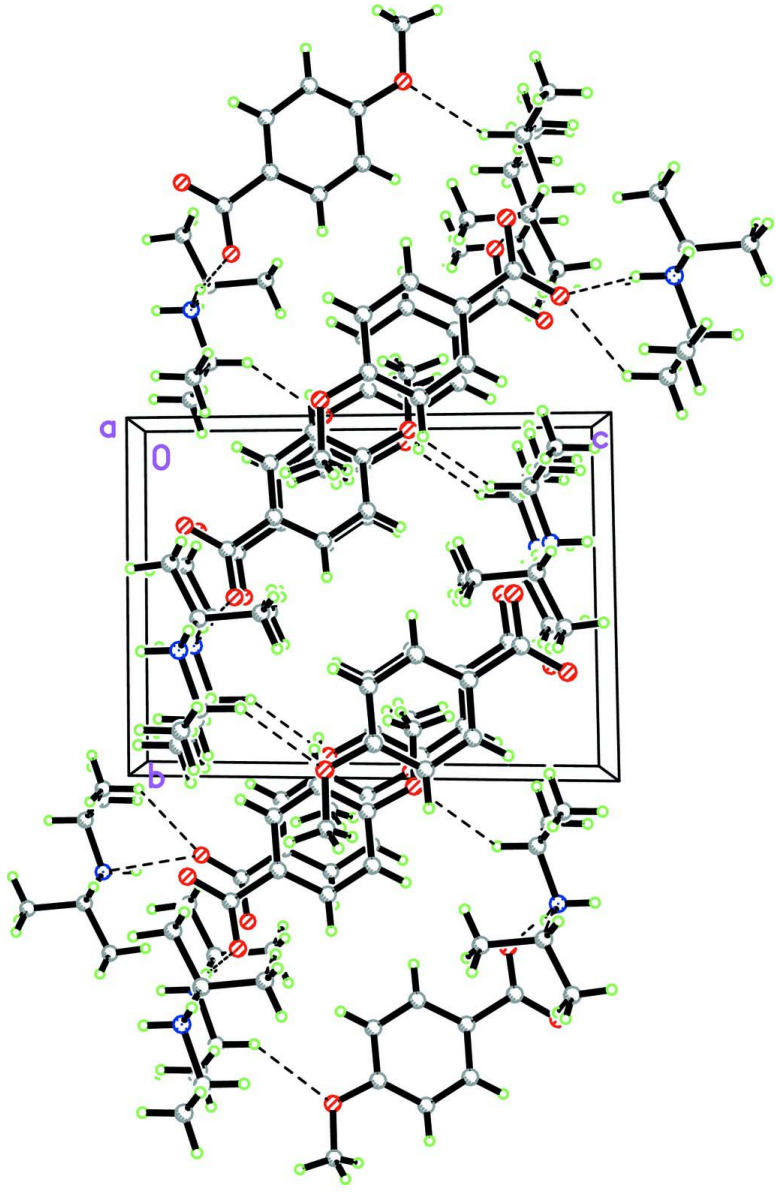

Figure 2

Packing of the title compound, stacking along the *a* axis. Dashed lines indicate hydrogen bonds.

Diisopropylammonium 4-methoxybenzoate

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Z = 2
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D_x = 1.100 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
θ = 6.2–55.3°
μ = 0.08 mm^{-1}
T = 293 K
Prism, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 28.5714 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.842, T_{max} = 1.000
7992 measured reflections
3501 independent reflections
1945 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 3.0°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.163
S = 1.04
3501 reflections
168 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 0.0936P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.20 e $Å^{-3}$
Extinction correction: *SHELXS97* (Sheldrick, 2008)
Extinction coefficient: 0.0000

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
C5	0.3367 (2)	0.7243 (2)	0.69733 (13)	0.0464 (4)
O2	0.4300 (2)	0.49545 (18)	0.78584 (12)	0.0787 (5)
C2	0.2819 (3)	0.8953 (2)	0.50734 (15)	0.0535 (5)
N1	0.2941 (2)	0.64829 (17)	0.11683 (11)	0.0526 (4)
H1A	0.3909	0.5944	0.1403	0.063*
H1B	0.3233	0.6510	0.0408	0.063*
C3	0.3349 (3)	0.7417 (2)	0.49873 (15)	0.0610 (5)
H3	0.3531	0.6951	0.4292	0.073*
C6	0.2841 (2)	0.8778 (2)	0.70400 (14)	0.0533 (5)
H6	0.2659	0.9246	0.7735	0.064*
O1	0.2546 (2)	0.96828 (17)	0.40924 (11)	0.0763 (5)
C8	0.3735 (3)	0.6323 (3)	0.79925 (16)	0.0570 (5)
C7	0.2573 (3)	0.9648 (2)	0.60979 (16)	0.0572 (5)
H7	0.2232	1.0688	0.6159	0.069*

O3	0.3476 (2)	0.70132 (19)	0.89014 (11)	0.0877 (5)
C4	0.3609 (3)	0.6570 (2)	0.59302 (15)	0.0541 (5)
H4	0.3951	0.5531	0.5866	0.065*
C12	0.2805 (3)	0.8068 (2)	0.15741 (17)	0.0678 (6)
H12	0.2411	0.8061	0.2400	0.081*
C1	0.2132 (3)	1.1280 (3)	0.4104 (2)	0.0807 (7)
H1C	0.0956	1.1550	0.4615	0.121*
H1D	0.2050	1.1645	0.3358	0.121*
H1E	0.3110	1.1729	0.4347	0.121*
C9	0.1253 (3)	0.5634 (3)	0.15227 (18)	0.0706 (6)
H9	0.0195	0.6204	0.1260	0.085*
C10	0.1664 (3)	0.4115 (3)	0.0961 (2)	0.0842 (7)
H10A	0.2012	0.4256	0.0157	0.126*
H10B	0.0565	0.3585	0.1142	0.126*
H10C	0.2677	0.3533	0.1227	0.126*
C13	0.1367 (4)	0.9106 (3)	0.1084 (2)	0.1088 (10)
H13A	0.1710	0.9092	0.0274	0.163*
H13B	0.1334	1.0121	0.1340	0.163*
H13C	0.0150	0.8760	0.1329	0.163*
C14	0.4734 (4)	0.8603 (3)	0.1257 (2)	0.0937 (8)
H14A	0.5591	0.7954	0.1610	0.141*
H14B	0.4676	0.9623	0.1507	0.141*
H14C	0.5162	0.8570	0.0451	0.141*
C11	0.0733 (4)	0.5482 (4)	0.2805 (2)	0.1119 (10)
H11A	0.1810	0.5040	0.3084	0.168*
H11B	−0.0262	0.4844	0.3013	0.168*
H11C	0.0323	0.6466	0.3127	0.168*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C5	0.0389 (9)	0.0635 (12)	0.0368 (9)	−0.0063 (8)	−0.0079 (7)	0.0001 (8)
O2	0.1004 (12)	0.0710 (10)	0.0741 (10)	−0.0030 (9)	−0.0451 (9)	0.0112 (8)
C2	0.0514 (11)	0.0669 (13)	0.0438 (10)	−0.0079 (9)	−0.0145 (8)	0.0084 (9)
N1	0.0586 (9)	0.0630 (10)	0.0373 (7)	−0.0025 (8)	−0.0151 (7)	0.0005 (6)
C3	0.0759 (14)	0.0706 (14)	0.0386 (10)	−0.0052 (11)	−0.0176 (9)	−0.0056 (9)
C6	0.0517 (11)	0.0665 (13)	0.0408 (10)	−0.0013 (9)	−0.0092 (8)	−0.0081 (8)
O1	0.0980 (11)	0.0798 (10)	0.0548 (8)	−0.0058 (8)	−0.0292 (8)	0.0167 (7)
C8	0.0519 (11)	0.0781 (15)	0.0445 (10)	−0.0100 (10)	−0.0173 (8)	0.0063 (9)
C7	0.0594 (12)	0.0556 (11)	0.0563 (11)	−0.0009 (9)	−0.0144 (9)	−0.0006 (9)
O3	0.1175 (13)	0.1062 (12)	0.0389 (8)	0.0002 (10)	−0.0225 (8)	0.0049 (8)
C4	0.0600 (11)	0.0559 (11)	0.0471 (10)	−0.0022 (9)	−0.0144 (8)	−0.0029 (8)
C12	0.0924 (16)	0.0619 (13)	0.0492 (11)	−0.0001 (12)	−0.0180 (11)	−0.0074 (9)
C1	0.0791 (16)	0.0799 (16)	0.0873 (16)	−0.0149 (13)	−0.0294 (12)	0.0331 (12)
C9	0.0568 (12)	0.0953 (17)	0.0628 (13)	−0.0142 (12)	−0.0156 (10)	−0.0068 (11)
C10	0.0764 (16)	0.0961 (18)	0.0887 (17)	−0.0278 (13)	−0.0257 (13)	−0.0091 (14)
C13	0.124 (2)	0.0868 (18)	0.108 (2)	0.0388 (17)	−0.0293 (18)	−0.0183 (15)
C14	0.116 (2)	0.0678 (15)	0.1050 (19)	−0.0272 (15)	−0.0328 (16)	0.0033 (13)

C11	0.109 (2)	0.157 (3)	0.0698 (16)	−0.069 (2)	0.0121 (14)	−0.0062 (16)

Geometric parameters (Å, º)

C5—C6	1.374 (2)	C12—C13	1.520 (3)
C5—C4	1.387 (2)	C12—H12	0.9800
C5—C8	1.509 (2)	C1—H1C	0.9600
O2—C8	1.244 (2)	C1—H1D	0.9600
C2—O1	1.372 (2)	C1—H1E	0.9600
C2—C7	1.375 (3)	C9—C10	1.505 (3)
C2—C3	1.376 (3)	C9—C11	1.523 (3)
N1—C12	1.494 (2)	C9—H9	0.9800
N1—C9	1.499 (2)	C10—H10A	0.9600
N1—H1A	0.9000	C10—H10B	0.9600
N1—H1B	0.9000	C10—H10C	0.9600
C3—C4	1.379 (2)	C13—H13A	0.9600
C3—H3	0.9300	C13—H13B	0.9600
C6—C7	1.389 (3)	C13—H13C	0.9600
C6—H6	0.9300	C14—H14A	0.9600
O1—C1	1.417 (3)	C14—H14B	0.9600
C8—O3	1.249 (2)	C14—H14C	0.9600
C7—H7	0.9300	C11—H11A	0.9600
C4—H4	0.9300	C11—H11B	0.9600
C12—C14	1.511 (3)	C11—H11C	0.9600
C6—C5—C4	117.94 (16)	O1—C1—H1D	109.5
C6—C5—C8	121.22 (16)	H1C—C1—H1D	109.5
C4—C5—C8	120.81 (17)	O1—C1—H1E	109.5
O1—C2—C7	124.49 (18)	H1C—C1—H1E	109.5
O1—C2—C3	115.47 (17)	H1D—C1—H1E	109.5
C7—C2—C3	120.04 (17)	N1—C9—C10	108.59 (17)
C12—N1—C9	117.80 (16)	N1—C9—C11	110.65 (17)
C12—N1—H1A	107.9	C10—C9—C11	111.9 (2)
C9—N1—H1A	107.9	N1—C9—H9	108.5
C12—N1—H1B	107.9	C10—C9—H9	108.5
C9—N1—H1B	107.9	C11—C9—H9	108.5
H1A—N1—H1B	107.2	C9—C10—H10A	109.5
C2—C3—C4	120.11 (17)	C9—C10—H10B	109.5
C2—C3—H3	119.9	H10A—C10—H10B	109.5
C4—C3—H3	119.9	C9—C10—H10C	109.5
C5—C6—C7	121.78 (17)	H10A—C10—H10C	109.5
C5—C6—H6	119.1	H10B—C10—H10C	109.5
C7—C6—H6	119.1	C12—C13—H13A	109.5
C2—O1—C1	118.28 (16)	C12—C13—H13B	109.5
O2—C8—O3	125.35 (18)	H13A—C13—H13B	109.5
O2—C8—C5	117.80 (17)	C12—C13—H13C	109.5
O3—C8—C5	116.83 (19)	H13A—C13—H13C	109.5
C2—C7—C6	119.14 (18)	H13B—C13—H13C	109.5

C2—C7—H7	120.4	C12—C14—H14A	109.5
C6—C7—H7	120.4	C12—C14—H14B	109.5
C3—C4—C5	120.98 (18)	H14A—C14—H14B	109.5
C3—C4—H4	119.5	C12—C14—H14C	109.5
C5—C4—H4	119.5	H14A—C14—H14C	109.5
N1—C12—C14	108.13 (18)	H14B—C14—H14C	109.5
N1—C12—C13	111.18 (18)	C9—C11—H11A	109.5
C14—C12—C13	111.6 (2)	C9—C11—H11B	109.5
N1—C12—H12	108.6	H11A—C11—H11B	109.5
C14—C12—H12	108.6	C9—C11—H11C	109.5
C13—C12—H12	108.6	H11A—C11—H11C	109.5
O1—C1—H1C	109.5	H11B—C11—H11C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O3^{i}	0.90	1.84	2.720 (2)	166
N1—H1*A*···O2^{ii}	0.90	1.83	2.721 (2)	169

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