Crystal structures and Hirshfeld surface analysis of 2-(adamantan-1-yl)-5-(4-fluorophenyl)-1,3,4-oxadiazole and 2-(adamantan-1-yl)-5-(4-chlorophenyl)-1,3,4-oxadiazole

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Abstract: The crystal structures of the title adamantane-oxadiazole hybrid compounds, C18H19FN2O (I) and C18H19ClN2O (II), are built up from an adamantane unit and a halogenophenyl ring, [X = F (I), Cl (Mb in position 5 on the central 1,3,4-oxadiazole unit. The molecular structures are very similar, only the relative orientation of the halogenophenyl ring in comparison with the central five membered ring differs slightly. In the crystals of both compounds, molecules are linked by pairs of C-H center dot center dot center dot N hydrogen bonds, forming inversion dimers with R-2(2)(12) ring motifs. In (I) the dimers are connected by C-H center dot center dot center dot F interactions, forming slabs lying parallel to the be plane. In (II), the dimers are linked by C-H center dot center dot center dot pi and offset pi-pi interactions [interplanar distance = 3.4039 (9) angstrom], forming layers parallel to (10 (1) over bar).

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The crystal structures of the title adamantane-oxadiazole hybrid compounds, C_{18}H_{19}FN_{2}O (I) and C_{18}H_{19}ClN_{2}O (II), are built up from an adamantane unit and a halogenophenyl ring, [X = F (I), Cl (II)], in position 5 on the central 1,3,4-oxadiazole unit. The molecular structures are very similar, only the relative orientation of the halogenophenyl ring in comparison with the central five-membered ring differs slightly. In the crystals of both compounds, molecules are linked by pairs of C—H···N hydrogen bonds, forming inversion dimers with R_2^2(12) ring motifs. In (I) the dimers are connected by C—H···F interactions, forming slabs lying parallel to the bc plane. In (II), the dimers are linked by C—H···π and offset π···π interactions [interplanar distance = 3.4039 (9) Å], forming layers parallel to (101).

1. Chemical context

Considerable attention has been devoted to adamantane derivatives, which have long been known for their diverse biological properties (Liu et al., 2011; Lamoureux & Artavia, 2010). In view of the pronounced lipophilicity of the adamantane cage, it has been observed that adamantyl-bearing compounds are characterized by high therapeutic indices (Wanka et al., 2013). Sixty years ago, the first adamantane-based drug, amantadine, was discovered to be an efficient therapy for the treatment of Influenza A infection (Davies et al., 1964; Togo et al., 1968). As a result of intensive research based on adamantane derivatives, the adamantane nucleus was further recognized as the key pharmacophore in several biologically active compounds. Among the major biological activities displayed by adamantane derivatives, the anti-HIV (El-Emam et al., 2004; Burstein et al., 1999; Balzarini et al., 2009), antibacterial (Protopopova et al., 2005; El-Emam et al., 2013; Kadi et al., 2010; Al-Abdullah et al., 2014; Al-Wahaibi et al., 2017), antifungal (Omar et al., 2010), anticancer (Sun et al., 2002), anti-diabetic (Villhauer et al., 2003; Augeri et al., 2005) and antimalarial (Dong et al., 2010) activities are the most interesting. In addition, 1,3,4-oxadiazole derivatives occupy a unique place in the field of medicinal chemistry as pharmacophores or auxophores possessing diverse pharmacological activities including antibacterial (Prakash et al., 2010; Ogata et al., 1971; Kadi et al., 2007), anticancer (Zhang et al.,...
2014), antiviral (Wu et al., 2015) and anti-inflammatory (Bansal et al., 2014) activities. We report herein on the crystal structure determinations of the title adamantane-oxadiazole hybrid molecules 2-(adamantan-1-yl)-5-(4-fluorophenyl)-1,3,4-oxadiazole (I) and 2-(adamantan-1-yl)-5-(4-chlorophenyl)-1,3,4-oxadiazole (II). The crystal structure of the 4-bromophenyl derivative has been reported previously (Alzoman et al., 2014), and after examination of the deposited CIF and transformation of the space group, from $P_2_1/c$ to $P_2_1/n$, it is found to be isotypic with compound (II).

2. Structural commentary

Compounds (I) and (II), are built up from a central 1,3,4-oxadiazole unit, an adamantane unit and a halogenophenyl group (Figs. 1 and 2, respectively). The C—N bonds in the oxadiazole rings have double-bond character [C7—N1 = 1.279 (5) and 1.292 (3) Å, and C8—N2 = 1.288 (5) and 1.288 (3) Å in (I) and (II), respectively], while the N—N and C—O bonds exhibit single-bond character [N1—N2 = 1.408 (4) and 1.417 (3) Å, C7—O1 = 1.366 (4) and 1.360 (2) Å, and C8—O1 = 1.369 (4) and 1.359 (2) Å in (I) and (II), respectively]. These geometrical parameters are very similar to those observed for similar compounds; see §5. Database survey.

As seen in Fig. 3, the molecular structures of compounds (I) and (II) are very similar. The largest difference is highlighted by the structural overlay plot, and comes from the relative orientation of the halogenophenyl group with respect to the oxadiazole ring. In compound (II), the rings are almost coplanar with their mean planes being inclined to each other by 9.5 (1)°, while in compound (I) the equivalent dihedral angle is 20.8 (2)°.

3. Supramolecular features

In the crystals of both compounds, molecules are linked by pairs of C—H···N hydrogen bonds, forming inversion dimers with $R_2^2(12)$ ring motifs (Tables 1 and 2, respectively). In the crystal of (I), the dimers are connected by C—H···F interactions, forming slabs lying parallel to the $bc$ plane (Fig. 4 and Table 1). In the crystal of (II), the dimers are linked by C—H···π and offset π···π interactions, forming layers lying parallel to the (10$ar{1}$) plane; see Fig. 5 and Table 2. The offset π···π interactions involve inversion-related 4-chlorophenyl rings (Cl—C6) with an intercentroid distance of 3.687 (1) Å, an interplanar distance of 3.404 (1) Å, and an offset of 1.418 Å. In Fig. 5 these interactions are represented by double-headed red arrows.

| Table 1 | Hydrogen-bond geometry (Å, °) for (I). |
|---------|--------------------------------------|
| $D—H···A$ | $D—H$ | $H···A$ | $D—A$ | $D—H···A$ |
| C3—H3···N1i | 0.95 | 2.56 | 3.383 (5) | 146 |
| C18—H18A···F1ii | 0.99 | 2.47 | 3.415 (5) | 139 |
| Symmetry codes: (i) $x+1$, $y+1$, $z+1$; (ii) $x+1$, $y+1$, $z+1$. |

| Table 2 | Hydrogen-bond geometry (Å, °) for (II). |
|---------|--------------------------------------|
| $D—H···A$ | $D—H$ | $H···A$ | $D—A$ | $D—H···A$ |
| C3—H3···N1i | 0.95 | 2.61 | 3.386 (3) | 139 |
| C12—H12A···Cl1i | 0.99 | 2.73 | 3.680 (3) | 160 |
| Symmetry codes: (i) $x+1$, $y+1$, $z+1$; (ii) $x+1$, $y+1$, $z+1$. |

Symmetry codes: (i) $x+1$, $y+1$, $z+1$; (ii) $x+1$, $y+1$, $z+1$.
4. Hirshfeld surface analysis

The Hirshfeld surfaces for (I) and (II) mapped over $d_{norm}$ were calculated using CrystalExplorer 17 (Turner et al., 2017) with the default setting of arbitrary units range. The characteristic bright-red spots near atoms H3, H18A, N1 and F1 (Fig. 6) confirm the previously mentioned C3—H3···N1$^i$ and C18—H18A···F1$^{ii}$ [symmetry codes: (i) $-x + 1$, $-y + 1$, $-z + 1$; (ii) $-x + 1$, $y - \frac{1}{2}$, $-z + \frac{3}{2}$] interatomic contacts in the crystal packing of (I). As expected, the same bright-red spots are observed near atoms H3 and N1 on the Hirshfeld surface of (II); see Fig. 7. The Hirshfeld surface mapped over the shape-index property elegantly illustrates the $\pi$--$\pi$ stacking and the C—H···$\pi$ interactions observed in the crystal packing of (II).
Two views are presented in Fig. 8. The π–π stacking between inversion-related 4-chlorophenyl rings (C1–C6) is indicated by the appearance of small blue regions surrounding a bright-red triangle within the six-membered ring (Fig. 8a), while the C12–H12A⋯·π(C1–C6)ii interaction [symmetry code: (ii) x + 1/2, −y + 1, z + 1/2] appears as a large red region within the ring (Fig. 8b).

5. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, February 2019; Groom et al., 2016) for the substructure 2-(adamantan-1-yl)-1,3,4-oxadiazole gave five hits. The crystal structures of three very similar compounds were reported in the last decade, namely 2-(adamantan-1-yl)-5-(4-nitrophenyl)-1,3,4-oxadiazole (CSD refcode LAPVOP; El-Emam et al., 2012), which has an NO2 group on the phenyl ring (in the title compounds. The 4-substituted phenyl rings are inclined to the oxadiazole ring by 0.0° in LAPVOP (as it lies in a mirror plane), 3.01° and 3.31° in the two independent molecules of SIKKAA and 10.44° in SOSXIJ. In the title compounds the corresponding dihedral angle is 20.8° for compound (I) and 9.5° for compound (II).

6. Synthesis and crystallization

Compounds (I) and (II) were synthesized via condensation of adamantane-1-carboxylic acid with 4-fluorobenzohydrazide, or 4-chlorobenzohydrazide in the presence of phosphorus oxychloride, as described previously (Kadi et al., 2007). Colourless plate-like crystals of compound (I) and colourless needle-like crystals of compound (II) were obtained by slow evaporation of CHCl3:EtOH (1:1 v:v) solutions at room temperature.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were placed in

| Experimental details. | (I) | (II) |
|-----------------------|-----|-----|
| Chemical formula      | C18H19FN2O | C18H19ClN2O |
| Crystal data, data collection and structure refinement details | | |
| No. of measured, independent and observed [F > 2σ(I)] reflections | 13058, 2903, 2578 | 14318, 3217, 3052 |
| Rint | 0.030 | 0.023 |
| R1, wR2 | 0.080, 0.233, 1.23 | 0.061, 0.167, 1.08 |
| No. of reflections | 3217 | |
| No. of parameters | 199 | 199 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained |
| Δρobs, Δρmax (e Å⁻³) | 0.47, –0.38 | 0.81, –0.26 |

The reduced cell of SOSXIJ indicates that it is isotypic with compound (II). Compound LAPVOP resides on a mirror plane, while compound SIKKAA crystallizes with two independent molecules in the asymmetric unit. The geometrical parameters of the oxadiazole rings are similar to those reported above for the title compounds. The 4-substituted phenyl rings are inclined to the oxadiazole ring by 0.0° in LAPVOP (as it lies in a mirror plane), 3.01° and 3.31° in the two independent molecules of SIKKAA and 10.44° in SOSXIJ. In the title compounds the corresponding dihedral angle is 20.8° (2°) for compound (I) and 9.5 (1°) for compound (II).
calculated positions and treated as riding atoms: C—H = 0.95–1.00 Å with $U_{iso} = 1.2U_{eq}$(C).

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Crystal structures and Hirshfeld surface analysis of 2-(adamantan-1-yl)-5-(4-fluorophenyl)-1,3,4-oxadiazole and 2-(adamantan-1-yl)-5-(4-chlorophenyl)-1,3,4-oxadiazole

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Computing details
For both structures, data collection: CrysAlis PRO (Rigaku OD, 2019); cell refinement: CrysAlis PRO (Rigaku OD, 2019); data reduction: CrysAlis PRO (Rigaku OD, 2019); program(s) used to solve structure: ShelXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL (Sheldrick, 2015b); molecular graphics: Mercury (Macrae et al., 2008); software used to prepare material for publication: OLEX2 (Dolomanov et al., 2009).

2-(Adamantan-1-yl)-5-(4-fluorophenyl)-1,3,4-oxadiazole (I)

Crystal data
C_{18}H_{19}FN_{2}O
F(000) = 632
D_{x} = 1.382 Mg m^{-3}
Mr = 298.35
Monoclinic, P2_{1}/c
Cu Kα radiation, λ = 1.54184 Å
a = 18.2525 (4) Å
b = 7.07855 (16) Å
θ = 4.9–78.5°
c = 11.2207 (2) Å
μ = 0.78 mm^{-1}
β = 98.556 (2)°
T = 160 K
V = 1433.59 (6) Å^{3}
Plate, colourless
Z = 4
0.18 × 0.15 × 0.02 mm

Data collection
XtaLAB Synergy, Dualflex, Pilatus 200K
diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 5.8140 pixels mm^{-1}
ω scans
Absorption correction: analytical
(CrysAlisPro; Rigaku OD, 2019)
T_{min} = 0.921, T_{max} = 0.990
13058 measured reflections
2903 independent reflections
2578 reflections with I > 2σ(I)
R_{int} = 0.030
θ_{max} = 74.5°, θ_{min} = 4.9°
h = −22→22
k = −8→8
l = −11→14

Refinement
Refinement on F^{2}
Least-squares matrix: full
R[F^{2} > 2σ(F^{2})] = 0.080
wR(F^{2}) = 0.233
S = 1.23
2903 reflections
199 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
w = 1/[σ^{2}(F_{o}^{2}) + (0.0572P)^{2} + 6.0123P]
where P = (F_{o}^{2} + 2F_{c}^{2})/3

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Supporting Information

\((\Delta/\sigma)_{\text{max}} < 0.001\)
\(\Delta \rho_{\text{max}} = 0.47 \text{ e Å}^{-3}\)

\(\Delta \rho_{\text{min}} = -0.38 \text{ e Å}^{-3}\)

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     | \(U_{\text{iso}}/U_{\text{eq}}\) |
|-----|-------|-------|-------|-----------------|
| C1  | 0.6397(2) | 0.5834(6) | 0.8751(3) | 0.0220(8) |
| C2  | 0.6287(2) | 0.5485(6) | 0.7528(3) | 0.0218(8) |
| H2  | 0.669009 | 0.519350 | 0.711237 | 0.026* |
| C3  | 0.5568(2) | 0.5574(5) | 0.6928(3) | 0.0189(7) |
| H3  | 0.547397 | 0.536452 | 0.608242 | 0.023* |
| C4  | 0.4979(2) | 0.5973(5) | 0.7558(3) | 0.0178(7) |
| C5  | 0.5114(2) | 0.6345(5) | 0.8784(3) | 0.0201(8) |
| H5  | 0.471482 | 0.664740 | 0.920495 | 0.024* |
| C6  | 0.5836(2) | 0.6276(6) | 0.9397(3) | 0.0234(8) |
| H6  | 0.593767 | 0.652639 | 1.023700 | 0.028* |
| C7  | 0.42268(19) | 0.5993(5) | 0.6869(3) | 0.0188(7) |
| C8  | 0.3054(2) | 0.5755(5) | 0.6523(3) | 0.0194(8) |
| C9  | 0.22741(19) | 0.5532(5) | 0.6776(3) | 0.0188(8) |
| C10 | 0.2034(2) | 0.7286(6) | 0.7450(4) | 0.0229(8) |
| H10A | 0.235907 | 0.742685 | 0.823383 | 0.027* |
| H10B | 0.208148 | 0.843843 | 0.696746 | 0.027* |
| C11 | 0.1226(2) | 0.7041(6) | 0.7656(4) | 0.0249(9) |
| H11 | 0.107002 | 0.816945 | 0.809285 | 0.030* |
| C12 | 0.0729(2) | 0.6855(7) | 0.6436(4) | 0.0280(9) |
| H12A | 0.020522 | 0.672769 | 0.656054 | 0.034* |
| H12B | 0.077248 | 0.800506 | 0.594894 | 0.034* |
| C13 | 0.0958(2) | 0.5124(6) | 0.5766(3) | 0.0261(9) |
| H13 | 0.063156 | 0.501154 | 0.496999 | 0.031* |
| C14 | 0.1769(2) | 0.5336(6) | 0.5561(3) | 0.0241(8) |
| H14A | 0.191844 | 0.421626 | 0.512660 | 0.029* |
| H14B | 0.181982 | 0.646678 | 0.506007 | 0.029* |
| C15 | 0.1155(2) | 0.5267(7) | 0.8408(4) | 0.0282(9) |
| H15A | 0.147857 | 0.538200 | 0.919522 | 0.034* |
| H15B | 0.063748 | 0.512872 | 0.855987 | 0.034* |
| C16 | 0.1378(2) | 0.3532(6) | 0.7743(4) | 0.0264(9) |
| H16 | 0.132697 | 0.237763 | 0.823688 | 0.032* |
| C17 | 0.0881(2) | 0.3342(6) | 0.6516(4) | 0.0282(9) |
| H17A | 0.102861 | 0.221647 | 0.608557 | 0.034* |
| H17B | 0.035805 | 0.318109 | 0.663834 | 0.034* |
| C18 | 0.2193(2) | 0.3748(6) | 0.7544(4) | 0.0242(8) |
| H18A | 0.234847 | 0.261751 | 0.712615 | 0.029* |
| H18B | 0.251650 | 0.386012 | 0.833140 | 0.029* |
|  | F1 | N1 | N2 | O1 |
|---|---|---|---|---|
| x | 0.71024 (12) | 0.40489 (17) | 0.32721 (18) | 0.36296 (13) |
| y | 0.5714 (4) | 0.6139 (5) | 0.5975 (5) | 0.5751 (4) |
| z | 0.9363 (2) | 0.5727 (3) | 0.5493 (3) | 0.7457 (2) |
| U11 | 0.0321 (6) |

**Atomic displacement parameters (Å²)**

| Atom | U11  | U22  | U33  | U12  | U13  | U23  |
|------|------|------|------|------|------|------|
| C1   | 0.0185 (18) | 0.0220 (19) | 0.0239 (19) | -0.0016 (15) | -0.0015 (14) | 0.0036 (15) |
| C2   | 0.0179 (17) | 0.0239 (19) | 0.0245 (19) | -0.0014 (15) | 0.0059 (14) | 0.0014 (15) |
| C3   | 0.0218 (18) | 0.0180 (17) | 0.0177 (17) | 0.0000 (14) | 0.0055 (14) | -0.0012 (13) |
| C4   | 0.0152 (16) | 0.0155 (16) | 0.0232 (17) | -0.0024 (13) | 0.0048 (13) | 0.0008 (14) |
| C5   | 0.0199 (17) | 0.0201 (18) | 0.0217 (18) | 0.0007 (14) | 0.0083 (14) | 0.0003 (14) |
| C6   | 0.028 (2) | 0.0220 (19) | 0.0204 (18) | -0.0023 (16) | 0.0029 (15) | -0.0004 (15) |
| C7   | 0.0170 (17) | 0.0187 (17) | 0.0220 (18) | -0.0004 (14) | 0.0074 (14) | 0.0000 (14) |
| C8   | 0.0182 (17) | 0.0217 (19) | 0.0178 (17) | 0.0005 (14) | 0.0014 (13) | -0.0002 (14) |
| C9   | 0.0163 (17) | 0.0260 (19) | 0.0141 (16) | 0.0021 (14) | 0.0015 (13) | 0.0001 (14) |
| C10  | 0.0163 (18) | 0.027 (2) | 0.0257 (19) | -0.0027 (15) | 0.0034 (14) | -0.0046 (16) |
| C11  | 0.0153 (17) | 0.034 (2) | 0.027 (2) | 0.0003 (16) | 0.0061 (14) | -0.0057 (17) |
| C12  | 0.0159 (18) | 0.039 (2) | 0.029 (2) | 0.0032 (17) | 0.0029 (15) | 0.0023 (18) |
| C13  | 0.0170 (18) | 0.041 (2) | 0.0191 (18) | -0.0018 (16) | -0.0021 (14) | -0.0039 (17) |
| C14  | 0.0179 (18) | 0.038 (2) | 0.0161 (17) | -0.0002 (16) | 0.0018 (14) | -0.0001 (16) |
| C15  | 0.0197 (18) | 0.045 (3) | 0.0201 (19) | -0.0023 (17) | 0.0047 (14) | -0.0018 (18) |
| C16  | 0.0197 (18) | 0.031 (2) | 0.030 (2) | -0.0026 (16) | 0.0057 (15) | 0.0047 (17) |
| C17  | 0.0205 (19) | 0.034 (2) | 0.030 (2) | -0.0060 (17) | 0.0046 (16) | -0.0061 (18) |
| C18  | 0.0211 (18) | 0.029 (2) | 0.0233 (19) | 0.0043 (16) | 0.0051 (15) | 0.0048 (16) |
| F1   | 0.0198 (11) | 0.0465 (16) | 0.0278 (12) | -0.0006 (10) | -0.0032 (9) | 0.0031 (11) |
| N1   | 0.0194 (15) | 0.0318 (18) | 0.0207 (16) | 0.0022 (13) | 0.0061 (12) | 0.0008 (14) |
| N2   | 0.0202 (16) | 0.0366 (19) | 0.0171 (15) | 0.0020 (14) | 0.0044 (12) | 0.0013 (14) |
| O1   | 0.0148 (12) | 0.0288 (14) | 0.0146 (12) | -0.0007 (10) | 0.0036 (9) | -0.0009 (10) |

**Geometric parameters (Å, °)**

| Bond | Distance | Angle |
|------|----------|-------|
| C1—C2 | 1.380 (5) | C11—H11 | 1.0000 |
| C1—C6 | 1.376 (5) | C11—C12 | 1.532 (6) |
| C1—F1 | 1.369 (4) | C11—C15 | 1.529 (6) |
| C2—H2 | 0.9500 | C12—H12A | 0.9900 |
| C2—C3 | 1.384 (5) | C12—H12B | 0.9900 |
| C3—H3 | 0.9500 | C12—C13 | 1.528 (6) |
| C3—C4 | 1.400 (5) | C13—H13 | 1.0000 |
| C4—C5 | 1.386 (5) | C13—C14 | 1.539 (5) |
| C4—C7 | 1.472 (5) | C13—C17 | 1.535 (6) |
| C5—H5 | 0.9500 | C14—H14A | 0.9900 |
| C5—C6 | 1.394 (5) | C14—H14B | 0.9900 |
| C6—H6 | 0.9500 | C15—H15A | 0.9900 |
| C7—N1 | 1.279 (5) | C15—H15B | 0.9900 |
| C7—O1 | 1.366 (4) | C15—C16 | 1.523 (6) |
| C8—C9 | 1.500 (5) | C16—H16 | 1.0000 |

*Acta Cryst. (2019). E75, 611-615*
C8—N2 1.288 (5)  C16—C17 1.538 (6)  
C8—O1 1.369 (4)  C16—C18 1.544 (5)  
C9—C10 1.550 (5)  C17—H17A 0.9900  
C9—C14 1.534 (5)  C17—H17B 0.9900  
C9—C18 1.548 (5)  C18—H18A 0.9900  
C10—H10A 0.9900  C18—H18B 0.9900  
C10—H10B 0.9900  N1—N2 1.408 (4)  
C10—C11 1.537 (5)  

C6—C1—C2 123.8 (4)  H12A—C12—H12B 108.2  
F1—C1—C2 118.3 (3)  C13—C12—C11 109.8 (3)  
F1—C1—C6 117.9 (3)  C13—C12—H12B 109.7  
C1—C2—C3 121.2  C13—C12—H12A 109.7  
C1—C2—C3 117.5 (3)  C12—C13—C11 109.8 (3)  
C3—C2—H2 121.2  C12—C13—C14 109.6 (3)  
C2—C3—H3 119.8  C12—C13—C17 109.6 (3)  
C2—C3—C4 120.5 (3)  C14—C13—H13 109.5  
C3—C4—C3 119.8  C14—C13—C17 109.5  
C3—C4—C7 117.6 (3)  C17—C13—C14 109.3 (3)  
C5—C4—C3 120.2 (3)  C9—C14—C13 109.3 (3)  
C5—C4—C7 122.2 (3)  C9—C14—H14A 109.7  
C4—C5—H5 120.1  C9—C14—H14B 109.7  
C4—C5—C6 119.9 (3)  C13—C14—H14A 109.7  
C6—C5—C6 120.1  C13—C14—H14B 109.7  
C1—C6—C5 118.1 (3)  H14A—C14—H14B 108.2  
C1—C6—C6 121.0  C11—C15—C11 109.7  
C5—C6—C6 121.0  C11—C15—H15A 109.7  
N1—C7—C4 127.2 (3)  H15A—C15—H15B 108.2  
N1—C7—O1 113.1 (3)  C16—C15—C11 110.0 (3)  
O1—C7—C4 119.7 (3)  C16—C15—H15A 109.7  
N2—C8—C9 127.7 (3)  C16—C15—H15B 109.7  
N2—C8—O1 112.5 (3)  C15—C16—C16 109.4  
O1—C8—C9 119.8 (3)  C15—C16—C17 110.1 (3)  
C8—C9—C10 110.7 (3)  C15—C16—C17 108.9 (3)  
C8—C9—C14 107.7 (3)  C17—C16—C16 109.4  
C8—C9—C18 111.2 (3)  C17—C16—C18 109.5 (3)  
C14—C9—C10 109.3 (3)  C18—C16—H16 109.4  
C14—C9—C18 109.1 (3)  C13—C17—C16 109.2 (3)  
C18—C9—C10 108.9 (3)  C13—C17—C17 109.8  
C9—C10—H10A 109.8  C13—C17—H17A 109.8  
C9—C10—H10B 109.8  C16—C17—H17A 109.8  
H10A—C10—H10B 108.3  C16—C17—H17B 109.8  
C11—C10—C9 109.3 (3)  H17A—C17—H17B 108.3  
C11—C10—H10A 109.8  C9—C18—H18A 109.8  
C11—C10—H10B 109.8  C9—C18—H18B 109.8  
C10—C11—H11 109.4  C16—C18—C9 109.6 (3)  
C12—C11—C10 109.2 (3)  C16—C18—H18A 109.8  
C12—C11—H11 109.4  C16—C18—H18B 109.8
C15—C11—C10 109.7 (3)  
C15—C11—H11 109.4  
C15—C11—C12 109.6 (3)  
C11—C12—H12A 109.7  
C11—C12—H12B 109.7

C1—C2—C3—C4 −1.1 (6)  
C2—C1—C6—C5 1.1 (6)  
C2—C3—C4—C5 2.2 (6)  
C2—C3—C4—C7 −178.3 (3)  
C3—C4—C5—C6 −1.6 (6)  
C3—C4—C7—N1 −18.2 (6)  
C3—C4—C7—O1 158.6 (3)  
C4—C5—C6—C1 0.0 (6)  
C4—C7—N1—N2 176.5 (4)  
C4—C7—O1—C8 −176.9 (3)  
C5—C4—C7—N1 161.3 (4)  
C5—C4—C7—O1 −22.0 (5)  
C6—C1—C2—C3 −0.5 (6)  
C7—C4—C5—C6 178.9 (4)  
C7—N1—N2—C8 0.4 (4)  
C8—C9—C10—C11 178.1 (3)  
C8—C9—C14—C13 −179.4 (3)  
C8—C9—C18—C16 −177.9 (3)  
C9—C8—N2—N1 179.3 (4)  
C9—C8—O1—C7 −179.6 (3)  
C9—C10—C11—C12 −60.3 (4)  
C9—C10—C11—C15 59.8 (4)  
C10—C9—C14—C13 −59.2 (4)  
C10—C9—C18—C16 59.8 (4)  
C10—C11—C12—C13 60.7 (4)  
C10—C11—C15—C16 −60.9 (4)  
C11—C12—C13—C14 −60.0 (4)  
C11—C12—C13—C17 60.0 (4)

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|-----|------|-------|---------|
| C3—H3···N1i | 0.95 | 2.56 | 3.383 (5) | 146 |
| C18—H18A···F1ii | 0.99 | 2.47 | 3.415 (5) | 159 |

Symmetry codes: (i) −x+1, −y+1, −z+1; (ii) −x+1, y−1/2, −z+3/2.
2-(Adamantan-1-yl)-5-(4-chlorophenyl)-1,3,4-oxadiazole (II)

Crystal data

C₁₈H₁₉ClN₂O

Mr = 314.80

Monoclinic, P2₁/n

a = 13.08241 (19) Å

b = 6.49259 (9) Å

C = 18.5129 (3) Å

β = 105.5609 (16)°

V = 1514.83 (4) Å³

Z = 4

F(000) = 664

D_x = 1.380 Mg m⁻³

Cu Kα radiation, λ = 1.54184 Å

θ = 3.7–79.0°

µ = 2.25 mm⁻¹

T = 160 K

Needle, colourless

0.33 × 0.12 × 0.08 mm

Data collection

XtaLAB Synergy, Dualflex, Pilatus 200K diffractometer

Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 5.8140 pixels mm⁻¹

ω scans

Absorption correction: analytical

(CrysAlisPro; Rigaku OD, 2019)

T_min = 0.642, T_max = 0.870

14318 measured reflections

3217 independent reflections

3052 reflections with I > 2σ(I)

R_int = 0.023

θ_max = 78.9°, θ_min = 3.7°

h = −16→16

k = −7→8

l = −23→23

Refinement

Refinement on F²

Least-squares matrix: full

R[F² > 2σ(F²)] = 0.061

wR(F²) = 0.167

S = 1.08

3217 reflections

199 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ(Fo²) + (0.094P)² + 1.5575P]

where P = (Fo² + 2Fc²)/3

(Δ/σ)max < 0.001

Δρ_max = 0.81 e Å⁻³

Δρ_min = −0.26 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   | Uiso* / Ueq |
|-----|-----|-----|-----|------------|
| C1  | 0.42626 (17) | 0.6044 (4) | 0.35491 (12) | 0.0302 (5) |
| C2  | 0.40263 (17) | 0.4056 (4) | 0.37203 (12) | 0.0317 (5) |
| H2  | 0.333320 | 0.351478 | 0.352048 | 0.038* |
| C3  | 0.48137 (17) | 0.2855 (4) | 0.41883 (12) | 0.0279 (5) |
| H3  | 0.466239 | 0.148920 | 0.431206 | 0.034* |
| C4  | 0.58338 (16) | 0.3685 (3) | 0.44753 (11) | 0.0254 (4) |
| C5  | 0.60437 (17) | 0.5705 (3) | 0.43076 (12) | 0.0280 (5) |
| H5  | 0.672884 | 0.627166 | 0.451644 | 0.034* |
| C6  | 0.52611 (17) | 0.6897 (4) | 0.38380 (13) | 0.0302 (5) |
| H6 | 0.540617 | 0.826921 | 0.371688 | 0.036* |
| C7 | 0.66623 (17) | 0.2413 (3) | 0.49555 (12) | 0.0229 (4) |
| C8 | 0.81754 (16) | 0.1694 (3) | 0.56872 (11) | 0.0238 (4) |
| C9 | 0.92972 (16) | 0.2106 (3) | 0.61176 (11) | 0.0219 (4) |
| C10 | 0.93691 (16) | 0.3930 (4) | 0.66595 (12) | 0.0282 (5) |
| H10A | 0.897237 | 0.360738 | 0.703168 | 0.034* |
| H10B | 0.904931 | 0.517124 | 0.637722 | 0.034* |
| C11 | 1.05425 (18) | 0.4345 (4) | 0.70636 (13) | 0.0314 (5) |
| H11 | 1.059032 | 0.553003 | 0.741610 | 0.038* |
| C12 | 1.1016 (2) | 0.2426 (4) | 0.75071 (13) | 0.0333 (5) |
| H12A | 1.062078 | 0.209782 | 0.787976 | 0.040* |
| H12B | 1.176566 | 0.268774 | 0.778004 | 0.040* |
| C13 | 1.09521 (18) | 0.0597 (4) | 0.69691 (13) | 0.0319 (5) |
| H13 | 1.126743 | −0.065180 | 0.726092 | 0.038* |
| C14 | 0.97843 (17) | 0.0175 (3) | 0.65594 (12) | 0.0285 (5) |
| H14A | 0.938650 | −0.018439 | 0.692756 | 0.034* |
| H14B | 0.973710 | −0.100189 | 0.621181 | 0.034* |
| C15 | 1.11625 (17) | 0.4853 (3) | 0.64960 (14) | 0.0319 (5) |
| H15A | 1.191412 | 0.512639 | 0.676075 | 0.038* |
| H15B | 1.086479 | 0.610423 | 0.621095 | 0.038* |
| C16 | 1.10922 (16) | 0.3031 (4) | 0.59555 (13) | 0.0284 (5) |
| H16 | 1.149192 | 0.336599 | 0.557972 | 0.034* |
| C17 | 1.15702 (17) | 0.1113 (4) | 0.63970 (14) | 0.0330 (5) |
| H17A | 1.232475 | 0.136605 | 0.665944 | 0.040* |
| H17B | 1.153464 | −0.006047 | 0.604985 | 0.040* |
| C18 | 0.99249 (17) | 0.2645 (3) | 0.55507 (12) | 0.0231 (4) |
| H18A | 0.987062 | 0.149794 | 0.518988 | 0.028* |
| H18B | 0.961848 | 0.389182 | 0.526636 | 0.028* |
| C11 | 0.32838 (4) | 0.75434 (10) | 0.29606 (3) | 0.0384 (2) |
| N1 | 0.66468 (15) | 0.0461 (3) | 0.50869 (12) | 0.0348 (5) |
| N2 | 0.76544 (15) | −0.0012 (3) | 0.55744 (12) | 0.0330 (4) |
| O1 | 0.76044 (11) | 0.3299 (2) | 0.53130 (8) | 0.0254 (3) |

**Atomic displacement parameters (Å²)**

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0236 (10) | 0.0423 (13) | 0.0245 (10) | 0.0028 (9) | 0.0060 (8) | 0.0015 (9) |
| C2 | 0.0215 (9) | 0.0424 (13) | 0.0291 (10) | −0.0040 (9) | 0.0036 (8) | −0.0017 (9) |
| C3 | 0.0218 (10) | 0.0354 (11) | 0.0263 (10) | −0.0056 (8) | 0.0060 (8) | −0.0019 (8) |
| C4 | 0.0218 (9) | 0.0291 (11) | 0.0248 (9) | −0.0027 (8) | 0.0054 (7) | −0.0014 (8) |
| C5 | 0.0232 (9) | 0.0290 (11) | 0.0307 (10) | −0.0028 (8) | 0.0050 (8) | −0.0010 (8) |
| C6 | 0.0256 (10) | 0.0341 (11) | 0.0310 (11) | −0.0006 (9) | 0.0077 (8) | 0.0012 (9) |
| C7 | 0.0186 (9) | 0.0250 (10) | 0.0244 (10) | −0.0048 (7) | 0.0045 (8) | −0.0021 (7) |
| C8 | 0.0236 (9) | 0.0217 (10) | 0.0263 (9) | −0.0011 (8) | 0.0069 (8) | −0.0033 (8) |
| C9 | 0.0200 (9) | 0.0223 (9) | 0.0233 (9) | −0.0016 (7) | 0.0055 (7) | −0.0007 (7) |
| C10 | 0.0248 (10) | 0.0286 (11) | 0.0303 (10) | 0.0010 (8) | 0.0056 (8) | −0.0073 (8) |
| C11 | 0.0292 (11) | 0.0290 (11) | 0.0311 (11) | −0.0009 (9) | −0.0001 (8) | −0.0078 (9) |
| C12 | 0.0294 (11) | 0.0431 (14) | 0.0233 (10) | −0.0022 (9) | −0.0001 (9) | 0.0021 (8) |
|           | U^11 (Å^2) | U^22 (Å^2) | U^33 (Å^2) | U^12 (Å^2) | U^13 (Å^2) | U^23 (Å^2) |
|-----------|------------|------------|------------|------------|------------|------------|
| C13       | 0.0289 (11) | 0.0258 (11) | 0.0349 (11) | 0.0003 (9) | −0.0018 (9) | 0.0083 (9) |
| C14       | 0.0285 (10) | 0.0229 (10) | 0.0314 (10) | −0.0029 (8) | 0.0034 (8)  | 0.0052 (8)  |
| C15       | 0.0238 (10) | 0.0234 (10) | 0.0432 (12) | −0.0052 (8) | −0.0004 (9) | 0.0036 (9)  |
| C16       | 0.0205 (10) | 0.0332 (11) | 0.0322 (11) | −0.0003 (8) | 0.0081 (8)  | 0.0056 (9)  |
| C17       | 0.0251 (10) | 0.0296 (11) | 0.0413 (12) | 0.0057 (9)  | 0.0036 (9)  | 0.0000 (9)  |
| C18       | 0.0213 (9)  | 0.0254 (10) | 0.0225 (9)  | −0.0001 (7) | 0.0059 (8)  | 0.0018 (7)  |
| N1        | 0.0242 (3)  | 0.0543 (4)  | 0.0342 (3)  | 0.0096 (2)  | 0.0034 (2)  | 0.0102 (2)  |
| N2        | 0.0268 (9)  | 0.0279 (10) | 0.0437 (11) | −0.0052 (7) | −0.0007 (8) | 0.0024 (8)  |
| O1        | 0.0203 (7)  | 0.0236 (7)  | 0.0300 (7)  | −0.0035 (6) | 0.0030 (6)  | 0.0005 (6)  |

**Geometric parameters (Å, °)**

| Bond/Angle     | Length (Å) | Angle (°) |
|----------------|------------|-----------|
| C1—C2          | 1.384 (4)  |           |
| C1—C6          | 1.387 (3)  |           |
| C1—Cl1         | 1.740 (2)  |           |
| C2—H2          | 0.9500     |           |
| C2—C3          | 1.393 (3)  |           |
| C3—H3          | 0.9500     |           |
| C3—C4          | 1.405 (3)  |           |
| C4—C5          | 1.391 (3)  |           |
| C4—C7          | 1.460 (3)  |           |
| C5—H5          | 0.9500     |           |
| C5—C6          | 1.388 (3)  |           |
| C6—H6          | 0.9500     |           |
| C7—N1          | 1.292 (3)  |           |
| C7—O1          | 1.360 (2)  |           |
| C8—C9          | 1.494 (3)  |           |
| C8—N2          | 1.288 (3)  |           |
| C8—O1          | 1.359 (3)  |           |
| C9—C10         | 1.538 (3)  |           |
| C9—C14         | 1.539 (3)  |           |
| C9—C18         | 1.536 (3)  |           |
| C10—H10A       | 0.9900     |           |
| C10—H10B       | 0.9900     |           |
| C10—C11        | 1.540 (3)  |           |
| C2—C1—C6       | 122.0 (2)  | C11—C12—C13 | 109.73 (18) |
| C2—C1—Cl1      | 119.56 (17) | H12A—C12—H12B | 108.2 |
| C6—C1—Cl1      | 118.48 (19) | C13—C12—H12A | 109.7 |
| C1—C2—H2       | 120.3       | C13—C12—H12B | 109.7 |
| C3—C2—H2       | 120.3       | C12—C13—H13  | 109.5 |
| C2—C3—H3       | 120.3       | C14—C13—C12  | 109.36 (19) |
| C2—C3—C4       | 119.3 (2)   | C17—C13—C12  | 109.38 (19) |
| C4—C3—H3       | 120.3       | C17—C13—H13  | 109.5 |
| C3—C4—C7       | 119.2 (2)   | C17—C13—C14  | 109.69 (18) |
| C5—C4—C3       | 120.1 (2)   | C9—C14—H14A  | 109.8 |
C5—C4—C7 120.68 (19)  C9—C14—H14B 109.8
C4—C5—H5 119.7  C13—C14—C9 109.39 (17)
C6—C5—C4 120.6 (2)  C13—C14—H14A 109.8
C6—C5—H5 119.7  C13—C14—H14B 109.8
C1—C6—C5 118.6 (2)  H14A—C14—H14B 108.2
C1—C6—H6 120.7  C11—C15—H15A 109.8
C5—C6—H6 120.7  C11—C15—H15B 109.8
N1—C7—C4 128.6 (2)  C11—C15—C16 109.40 (18)
N1—C7—O1 112.39 (19)  H15A—C15—H15B 108.2
O1—C7—C4 119.03 (17)  C16—C15—H15A 109.8
N2—C8—C9 129.94 (19)  C16—C15—H15B 109.8
N2—C8—O1 112.47 (18)  C15—C16—H16 109.5
O1—C8—C9 117.48 (17)  C17—C16—H16 109.5
O1—C8—C9 111.42 (17)  C17—C16—C15 109.55 (18)
C8—C9—C10 110.16 (17)  C17—C16—H15B 109.8
C8—C9—C14 107.76 (17)  C13—C17—H17A 109.8
C10—C9—C14 109.67 (17)  C13—C17—H17B 109.8
C18—C9—C14 109.12 (17)  C16—C17—C13 109.39 (18)
C9—C10—H10A 109.8  C16—C17—H17A 109.8
C9—C10—H10B 109.8  C16—C17—H17B 109.8
C10—C11—C12 109.27 (17)  C15—C11—H11 110.36 (18)
H10A—C10—H10B 108.3  H18A—C18—H18B 108.1
C11—C10—H10A 109.8  C9—C18—H18A 109.6
C11—C10—H10B 109.8  C9—C18—H18B 109.6
C10—C11—H11 109.3  C16—C18—C9 110.41 (17)
C12—C11—C10 109.02 (19)  C16—C18—H18A 109.6
C12—C11—H11 109.3  C16—C18—H18B 109.6
C15—C11—C10 110.36 (18)  H18A—C18—H18B 108.1
C15—C11—H11 109.3  C7—N1—N2 105.90 (18)
C15—C11—C12 109.41 (19)  C8—N2—N1 106.14 (18)
C11—C12—H12A 109.7  C8—O1—C7 103.10 (16)
C11—C12—H12B 109.7

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C3—H3···N1i | 0.95 | 2.61 | 3.386 (3) | 139 |
| C12—H12A···Cg1ii | 0.99 | 2.73 | 3.680 (3) | 160 |

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