# organic compounds

# Four (*E,Z,E*)-1-(4-alkoxyphenyl)-6-(4-nitrophenyl)hexa-1,3,5-trienes

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The crystal structures of the four *E,Z,E* isomers of 1-(4-alkoxyphenyl)-6-(4-nitrophenyl)hexa-1,3,5-triene, namely (*E,Z,E*)-1-(4-methoxyphenyl)-6-(4-nitrophenyl)hexa-1,3,5-triene, $C_{19}H_{17}NO_3$, (*E,Z,E*)-1-(4-ethoxyphenyl)-6-(4-nitrophenyl)hexa-1,3,5-triene, $C_{20}H_{19}NO_3$, (*E,Z,E*)-1-(4-nitrophenyl)-6-(4-*n*-propoxyphenyl)hexa-1,3,5-triene, $C_{21}H_{21}NO_3$, and (*E,Z,E*)-1-(4-*n*-butoxyphenyl)-6-(4-nitrophenyl)hexa-1,3,5-triene, $C_{22}H_{23}NO_3$, have been determined. Intermolecular N···O dipole interactions between the nitro groups are observed for the methoxy derivative, while for the ethoxy derivative, two adjacent molecules are linked at both ends through N···O dipole–dipole interactions between the N atom of the nitro group and the O atom of the ethoxy group to form a supramolecular ring-like structure. In the crystal structures of the *n*-propoxy and *n*-butoxy derivatives, the shortest intermolecular distances are those between the two O atoms of the alkoxy groups. Thus, the nearest two molecules form an S-shaped supramolecular dimer in these crystal structures.

## Comment

π-Conjugated bent molecules are attracting increased attention at the current time (Yamaguchi *et al.*, 2005; Ros *et al.*, 2005). We have recently reported the crystal structures and photophysical properties of a series of (*E,E,E*)-1-(4-alkoxyphenyl)-6-(4-nitrophenyl)hexa-1,3,5-trienes, namely the methoxy, ethoxy, *n*-propoxy and *n*-butoxy compounds (Sonoda *et al.*, 2006). In the course of our study, we obtained single crystals of their *E,Z,E* isomers [(I)–(IV)], whose crystal structures we describe here. To the best of our knowledge, the crystal structure of 1,6-diphenylhexa-1,3,5-triene (DPH) having the *E,Z,E* configuration at the triene double bonds has not been reported. Our data can be compared with those for dibenzo[18]annulene incorporating two (*E,Z,E*)-DPH units (Michels *et al.*, 1994).

For compounds (I), (III) and (IV), only one independent molecule is present in the asymmetric unit, while for compound (II), two crystallographically independent molecules, *A* and *B*, are contained in the unit cell (Figs. 1–4). Selected geometric parameters for (I)–(IV) are given in Table 1.



(I)  $R = -Me$
(II)  $R = -CH_2Me$
(III)  $R = -CH_2CH_2Me$
(IV)  $R = -CH_2CH_2CH_2Me$
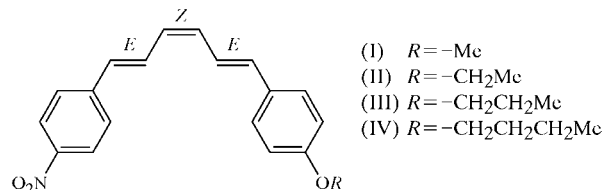
Bond-length alternation is one of the most important structural parameters that correlates closely with the electronic and optical properties of one-dimensional conjugated compounds, such as polyene and polyyne, since it strongly affects the band gaps of these molecules (Yang & Kertesz, 2006). In the present compounds, the averaged values of bond-
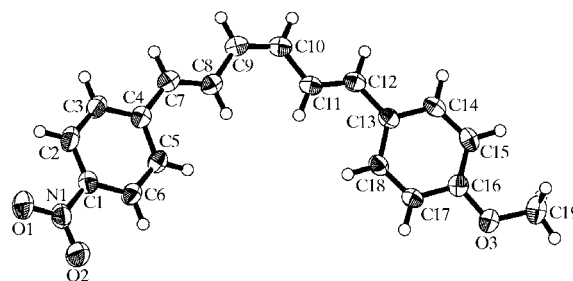


**Figure 1**
A view of the molecular structure and the atom-numbering scheme of the independent molecule in (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.
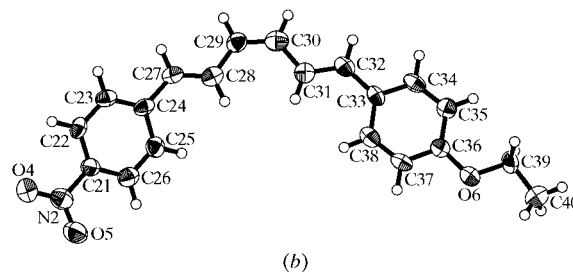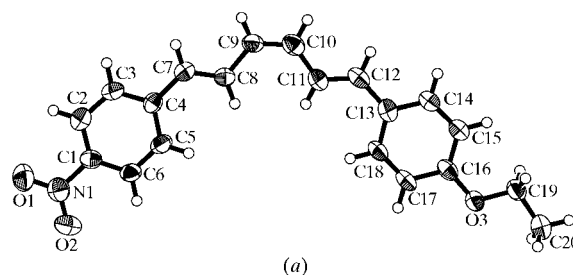


(*a*)



(*b*)

**Figure 2**
A view of the molecular structure and the atom-numbering scheme of the independent molecules in (II), *viz.* (*a*) molecule *A* and (*b*) molecule *B*. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

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length alternation ($\delta r$, the difference between C—C single- and C=C double-bond lengths) in the hexatriene chain are 0.107 Å for (I), 0.103 and 0.091 Å for molecules $A$ and $B$ of (II), respectively, 0.101 Å for (III), and 0.104 Å for (IV). The value of $\delta r$ for ($E$)-polyacetylene, a polyene with an infinite chain length, has been determined spectroscopically to be 0.08 Å (Yannoni & Clarke, 1983). The bond alternation is thus more distinctly observed in trienes (I)–(IV) than in polyacetylene, as expected. Interestingly, the single- and double-bond lengths and the resulting $\delta r$ values of (I)–(IV) are not greatly different from those of their $E,E,E$ counterparts. In the crystal structure of the $E,E,E$ isomer of (I), for example, the single-bond lengths are 1.434 (5)–1.460 (5) Å, the double-bond lengths are 1.333 (5)–1.345 (5) Å, and the values of $\delta r$ are 0.101 and 0.114 Å for the two crystallographically independent molecules (Sonoda *et al.*, 2006).

The geometry of the isolated molecule of (I) was optimized by *ab initio* calculations using the *GAUSSIAN03* program (Frisch *et al.*, 2004). The lengths of single bonds in the MP2/6–31G* (Møller & Plesset, 1934) level geometries (C4—C7 = 1.460 Å, C8—C9 = C10—C11 = 1.441 Å and C12—C13 = 1.459 Å) agree well with the values determined from the crystal structure, although the calculated lengths of the double bonds (C7=C8 = C11=C12 = 1.358 Å and C9=C10 = 1.364 Å) are slightly longer than those found in the crystal. The value of $\delta r$ obtained from the calculation (0.090 Å) is in reasonable agreement with that from the crystal structure determination. It should be noted that the calculation at the HF/6–31G* level yields a considerably large value of $\delta r$ (0.133 Å). A similar trend has been reported for polyacetylene oligomers (Choi *et al.*, 1997; Jacquemin *et al.*, 2005).

The internal C—C—C bond angles in the hexatriene chain are all somewhat wider than 120° for all structures, which minimizes the steric hindrance between the C5—H and C8—H atoms, between the C8—H and C11—H atoms, and between the C11—H and C18—H atoms.

The torsion angle of the single bond between the aromatic ring and the triene chain is different for each molecule. The C5—C4—C7—C8 angle [−0.7 (2)°] in (I) and the C25—C24—C27—C28 angle [20.9 (11)°] in (II) display the minimum and the maximum deviations from values of 0 or 180° in these molecules, respectively. The optimized geometry of an isolated molecule of (I) is such that the C5—C4—C7—C8 and C11—C12—C13—C18 torsion angles are −22.65 and −18.93°. *Ab initio* calculations of 4,4′-disubstituted DPHs show that the torsional potential is very shallow when the torsion angle is between −30 and 30° (Tsuzuki, 2003). It is therefore very probable that the torsion angle will have a different value depending on the packing force in each crystal. Other torsion angles in the triene chains are almost 0 or 180° for all four compounds, indicating that the triene planes are nearly planar for conjugation.

Figs. 5–8 show the crystal structures of (I)–(IV). For all compounds, neighboring molecules have a head-to-tail orientation. This results from donor–acceptor substitution on the rings, as the calculated dipole moment of (I) is 6.38 D (MP2/6–311G**//MP2/6–31G* level).
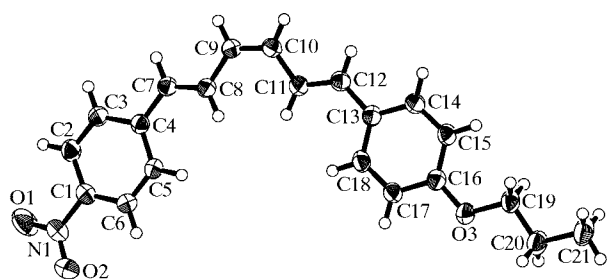


**Figure 3**
A view of the molecular structure and the atom-numbering scheme of the independent molecule in (III). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.



**Figure 4**
A view of the molecular structure and the atom-numbering scheme of the independent molecule in (IV). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.
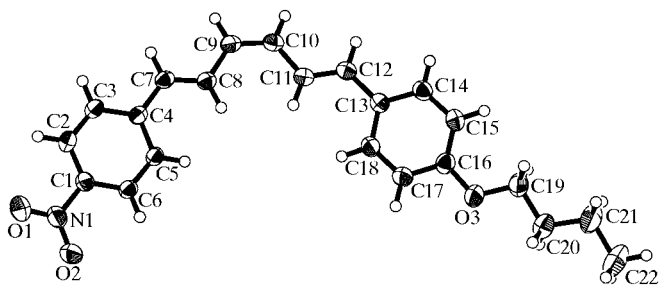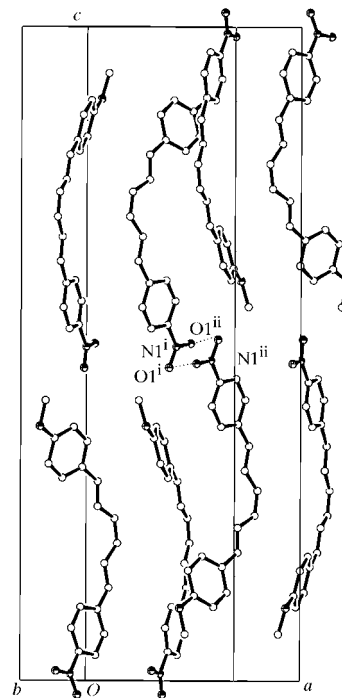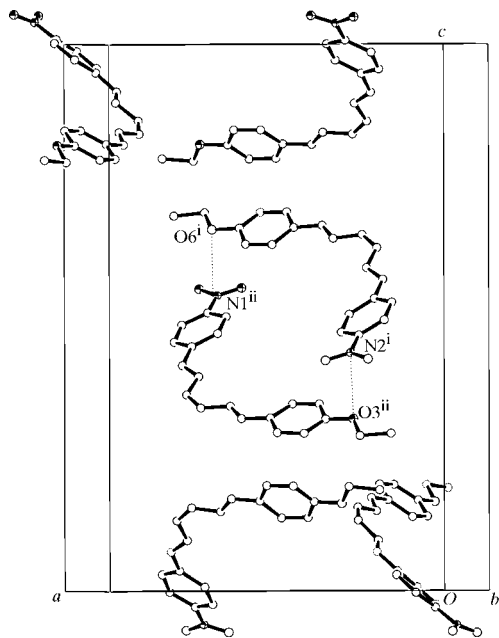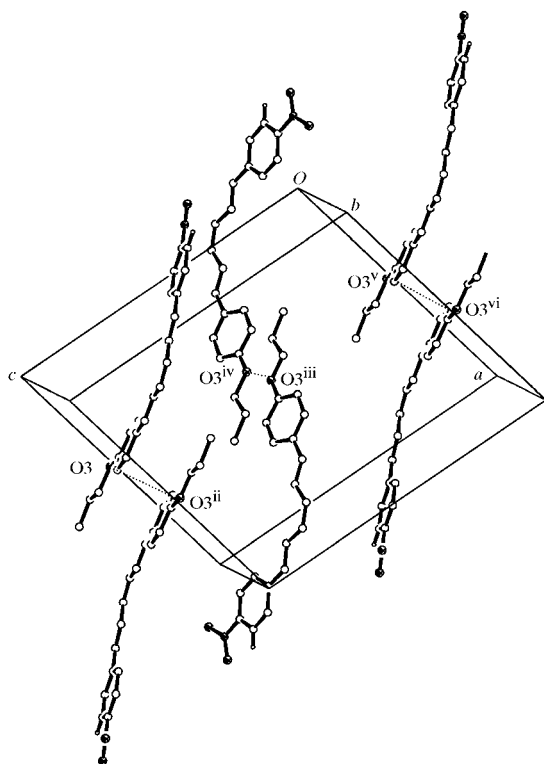


**Figure 5**
A partial view of the molecular packing in (I). Dotted lines indicate the shortest O···N intermolecular distances [O1$^{i}$···N1$^{ii}$ = 3.417 (2) Å; symmetry codes: (i) $-x + \frac{3}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (ii) $x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$].

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**Figure 6**
A partial view of the molecular packing in (II). Dotted lines indicate the intermolecular distances between the N atoms of the nitro groups and the O atoms of the ethoxy groups [O6$^i$···N1$^{ii}$ = 3.392 (9) Å and N2$^i$···O3$^{ii}$ = 3.427 (9) Å; symmetry codes: (i) $-x + 1$, $-y + 1$, $z + \frac{1}{2}$; (ii) $-x + 1$, $-y + 1$, $z - \frac{1}{2}$].

In the crystal structure of (I), attractive N···O interactions between the nitro groups are observed. The nearest two nitro groups are in a parallel arrangement, which allows the overlap of the N—O dipoles (Szezesna & Urbańczyk-Lipkowska, 2002; Zeller & Hunter, 2004). The parallel arrangement is also observed in the *E,E,E* isomer of (I); however, the shortest intermolecular distance between the N and O atoms in (I) [O1···N1$^{iii}$ = 3.417 (2) Å; symmetry code: (iii) $-x + 2$, $-y + 1$, $-z + 2$] is considerably larger than the N···O distance of 2.938 (4) Å in its *E,E,E* isomer (Sonoda *et al.*, 2006).

In the crystal structure of (II), two adjacent molecules are linked at both ends through N···O dipole interactions between the N atom of the nitro group and the O atom of the ethoxy group to form a supramolecular ring-like structure. The intermolecular distances between the N and O atoms are 3.392 (9) [O6···N1($x, y, z + 1$)] and 3.427 (9) Å [O3···N2($x, y, z + 1$)]. These supramolecular rings are piled up along the *c* axis. The least-squares plane defined by the molecule at ($x, y, z$) makes an angle of 56.47 (3)° with the least-squares plane defined by the molecule at ($x + \frac{1}{2}, -y, z$).

In the crystal structures of (III) and (IV), the shortest intermolecular distances are those between the two O atoms of the alkoxy groups: O3···O3($-x + 1$, $-y + 1$, $-z + 2$) = 4.284 (2) Å for (III), and O3···O3($-x$, $-y + 2$, $-z$) = 3.832 (2) Å for (IV). Thus, the nearest two molecules form an S-shaped supramolecular dimer in these crystal structures.
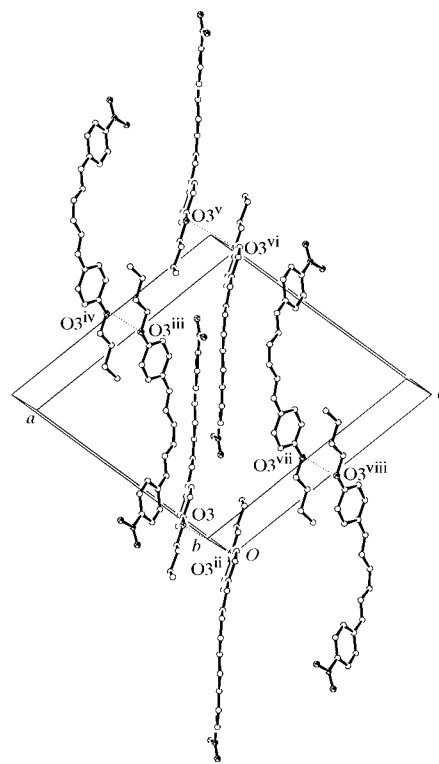


**Figure 7**
A partial view of the molecular packing in (III). Dotted lines indicate the shortest O···O intermolecular distances [O3···O3$^{ii}$ = O3$^{iii}$···O3$^{iv}$ = O3$^v$···O3$^{vi}$ = 4.284 (2) Å; symmetry codes: (ii) $-x + 1$, $-y + 1$, $-z + 2$; (iii) $-x + 1$, $y - \frac{1}{2}$, $-z + \frac{3}{2}$; (iv) $x$, $-y + \frac{1}{2}$, $z - \frac{1}{2}$; (v) $x, y, z - 1$; (vi) $-x + 1$, $-y + 1$, $-z + 1$].



**Figure 8**
A partial view of the molecular packing in (IV). Dotted lines indicate the shortest O···O intermolecular distances [O3···O3$^{ii}$ = O3$^{iii}$···O3$^{iv}$ = O3$^v$···O3$^{vi}$ = O3$^{vii}$···O3$^{viii}$ = 3.832 (2) Å; symmetry codes: (ii) $-x$, $-y + 2$, $-z$; (iii) $-x + 1$, $y - \frac{1}{2}$, $-z + \frac{1}{2}$; (iv) $x + 1$, $-y + \frac{3}{2}$, $z + \frac{1}{2}$; (v) $x + 1, y, z + 1$; (vi) $-x + 1$, $-y + 2$, $-z + 1$; (vii) $x$, $-y + \frac{3}{2}$, $z + \frac{1}{2}$; (viii) $-x$, $y - \frac{1}{2}$, $-z + \frac{1}{2}$].

## Experimental

Compounds (I)–(IV) were prepared by the Wittig reactions of the triphenylphosphonium salt of (E)-4-nitrocinnamyl bromide and (E)-4-alkoxycinnamaldehydes (Sonoda *et al.*, 2006). The reaction gave a mixture of E,Z,E and E,E,E isomers as a crude product, from which the E,E,E isomer was removed by recrystallization from toluene. Toluene was evaporated from the mother liquor under reduced pressure, and the resulting isomeric mixture (predominantly E,Z,E) was dissolved in an appropriate solvent [acetonitrile for (I) and dichloromethane–toluene for (II)–(IV)]. Crystals suitable for X-ray diffraction were obtained from these solutions by slow evaporation at room temperature in the dark. The melting points of (I)–(IV) could not be determined, probably because of thermal conversion to the E,E,E isomers in the solid state. $^1$H NMR (CDCl$_3$, 300 MHz): for (I), $\delta$ 8.20 (2H, *d*, *J* = 8.9 Hz, arom.), 7.58 (2H, *d*, *J* = 8.6 Hz, arom.), 7.44 (2H, *d*, *J* = 8.6 Hz, arom.), 7.24 (1H, *dd*, *J* = 15.8 and 11.6 Hz, triene), 6.90 (2H, *d*, *J* = 8.9 Hz, arom.), 6.56–6.68 (3H, *m*, triene), 6.36 [1H, apparently (app.) *t*, *J* = 11.1 Hz, triene], 6.21 (1H, app. *t*, *J* = 11.4 Hz, triene), 3.84 (3H, *s*, OCH$_3$); for (II), $\delta$ 8.19 (2H, *d*, *J* = 8.8 Hz, arom.), 7.58 (2H, *d*, *J* = 8.8 Hz, arom.), 7.43 (2H, *d*, *J* = 8.9 Hz, arom.), 7.23 (1H, *dd*, *J* = 15.4 and 11.5 Hz, triene), 6.89 (2H, *d*, *J* = 8.8 Hz, arom.), 6.56–6.67 (3H, *m*, triene), 6.36 (1H, app. *t*, *J* = 11.3 Hz, triene), 6.20 (1H, app. *t*, *J* = 11.4 Hz, triene), 4.07 (2H, *q*, *J* = 7.0 Hz, OCH$_2$), 1.43 (3H, *t*, *J* = 7.0 Hz, CH$_3$); for (III), $\delta$ 8.20 (2H, *d*, *J* = 8.7 Hz, arom.), 7.58 (2H, *d*, *J* = 8.8 Hz, arom.), 7.43 (2H, *d*, *J* = 8.7 Hz, arom.), 7.23 (1H, *dd*, *J* = 15.4 and 10.9 Hz, triene), 6.89 (2H, *d*, *J* = 8.8 Hz, arom.), 6.56–6.67 (3H, *m*, triene), 6.36 (1H, app. *t*, *J* = 11.1 Hz, triene), 6.20 (1H, app. *t*, *J* = 11.0 Hz, triene), 3.94 (2H, *t*, *J* = 6.6 Hz, OCH$_2$), 1.76–1.87 (2H, *m*, CH$_2$Me), 1.04 (3H, *t*, *J* = 7.4 Hz, CH$_3$); for (IV), $\delta$ 8.20 (2H, *d*, *J* = 8.5 Hz, arom.), 7.58 (2H, *d*, *J* = 8.9 Hz, arom.), 7.42 (2H, *d*, *J* = 8.7 Hz, arom.), 7.23 (1H, *dd*, *J* = 15.5 and 11.3 Hz, triene), 6.89 (2H, *d*, *J* = 8.6 Hz, arom.), 6.56–6.67 (3H, *m*, triene), 6.36 (1H, app. *t*, *J* = 11.0 Hz, triene), 6.20 (1H, app. *t*, *J* = 11.0 Hz, triene), 3.99 (2H, *t*, *J* = 6.4 Hz, OCH$_2$), 1.73–1.83 (2H, *m*, CH$_2$Et), 1.44–1.57 (2H, *m*, CH$_2$Me), 0.99 (3H, *t*, *J* = 7.4 Hz, CH$_3$).

## Compound (I)

### Crystal data

| | |
|---|---|
| C$_{19}$H$_{17}$NO$_3$ | $Z = 8$ |
| $M_r = 307.34$ | $D_x = 1.297$ Mg m$^{-3}$ |
| Orthorhombic, *Pbcn* | Mo $K\alpha$ radiation |
| $a = 13.0541$ (11) Å | $\mu = 0.09$ mm$^{-1}$ |
| $b = 6.9672$ (6) Å | $T = 183$ (2) K |
| $c = 34.604$ (3) Å | Rectangular, orange |
| $V = 3147.2$ (5) Å$^3$ | $0.30 \times 0.10 \times 0.04$ mm |

### Data collection

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 18236 measured reflections |
| $\varphi$ and $\omega$ scans | 3715 independent reflections |
| | 2905 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $R_{int} = 0.026$ |
| $T_{min} = 0.914$, $T_{max} = 0.997$ | $\theta_{max} = 28.3°$ |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0827P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.043$ | $+ 0.2636P]$ |
| $wR(F^2) = 0.136$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.07$ | $(\Delta/\sigma)_{max} = 0.005$ |
| 3715 reflections | $\Delta\rho_{max} = 0.24$ e Å$^{-3}$ |
| 209 parameters | $\Delta\rho_{min} = -0.19$ e Å$^{-3}$ |
| H-atom parameters constrained | |

## Compound (II)

### Crystal data

| | |
|---|---|
| C$_{20}$H$_{19}$NO$_3$ | $Z = 8$ |
| $M_r = 321.36$ | $D_x = 1.265$ Mg m$^{-3}$ |
| Orthorhombic, *Pca2$_1$* | Mo $K\alpha$ radiation |
| $a = 18.914$ (9) Å | $\mu = 0.09$ mm$^{-1}$ |
| $b = 6.880$ (3) Å | $T = 183$ (2) K |
| $c = 25.927$ (11) Å | Rectangular, orange |
| $V = 3374$ (3) Å$^3$ | $0.30 \times 0.10 \times 0.03$ mm |

### Data collection

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 11787 measured reflections |
| $\varphi$ and $\omega$ scans | 2972 independent reflections |
| | 1583 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick 1996) | $R_{int} = 0.135$ |
| $T_{min} = 0.933$, $T_{max} = 0.998$ | $\theta_{max} = 25.0°$ |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.064$ | $w = 1/[\sigma^2(F_o^2) + (0.0531P)^2]$ |
| $wR(F^2) = 0.155$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.92$ | $(\Delta/\sigma)_{max} = 0.003$ |
| 2972 reflections | $\Delta\rho_{max} = 0.19$ e Å$^{-3}$ |
| 435 parameters | $\Delta\rho_{min} = -0.20$ e Å$^{-3}$ |

## Compound (III)

### Crystal data

| | |
|---|---|
| C$_{21}$H$_{21}$NO$_3$ | $Z = 4$ |
| $M_r = 335.39$ | $D_x = 1.251$ Mg m$^{-3}$ |
| Monoclinic, *P2$_1$/c* | Mo $K\alpha$ radiation |
| $a = 15.3615$ (11) Å | $\mu = 0.08$ mm$^{-1}$ |
| $b = 6.8341$ (5) Å | $T = 223$ (2) K |
| $c = 17.6625$ (12) Å | Rectangular, red |
| $\beta = 106.215$ (1)° | $0.45 \times 0.20 \times 0.20$ mm |
| $V = 1780.5$ (2) Å$^3$ | |

### Data collection

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 10440 measured reflections |
| $\varphi$ and $\omega$ scans | 4007 independent reflections |
| | 3307 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $R_{int} = 0.023$ |
| $T_{min} = 0.873$, $T_{max} = 0.984$ | $\theta_{max} = 28.3°$ |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0623P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.041$ | $+ 0.288P]$ |
| $wR(F^2) = 0.116$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.03$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 4007 reflections | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| 227 parameters | $\Delta\rho_{min} = -0.23$ e Å$^{-3}$ |
| H-atom parameters constrained | |

## Compound (IV)

### Crystal data

| | |
|---|---|
| C$_{22}$H$_{23}$NO$_3$ | $Z = 4$ |
| $M_r = 349.41$ | $D_x = 1.222$ Mg m$^{-3}$ |
| Monoclinic, *P2$_1$/c* | Mo $K\alpha$ radiation |
| $a = 17.0571$ (10) Å | $\mu = 0.08$ mm$^{-1}$ |
| $b = 6.7244$ (4) Å | $T = 183$ (2) K |
| $c = 17.2095$ (10) Å | Rectangular, orange |
| $\beta = 105.884$ (1)° | $0.40 \times 0.15 \times 0.04$ mm |
| $V = 1898.54$ (19) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 11363 measured reflections |
| $\varphi$ and $\omega$ scans | 4309 independent reflections |
| Absorption correction: multi-scan ($SADABS$; Sheldrick, 1996) | 3596 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.888$, $T_{max} = 0.997$ | $R_{int} = 0.019$ |
| | $\theta_{max} = 28.2°$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0687P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | $+ 0.3548P]$ |
| $wR(F^2) = 0.130$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.05$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 4309 reflections | $\Delta\rho_{max} = 0.21$ e Å$^{-3}$ |
| 236 parameters | $\Delta\rho_{min} = -0.26$ e Å$^{-3}$ |
| H-atom parameters constrained | |

**Table 1**
Selected geometric parameters (Å, °) for compounds (I)–(IV).

| | (I) | (II) | (III) | (IV) |
|---|---|---|---|---|
| C4—C7 | 1.455 (2) | 1.459 (10) | 1.4535 (15) | 1.4564 (17) |
| C7—C8 | 1.339 (2) | 1.347 (10) | 1.3422 (15) | 1.3415 (16) |
| C8—C9 | 1.4369 (19) | 1.447 (10) | 1.4366 (16) | 1.4400 (17) |
| C9—C10 | 1.345 (2) | 1.348 (10) | 1.3514 (16) | 1.3486 (17) |
| C10—C11 | 1.4397 (19) | 1.446 (10) | 1.4405 (16) | 1.4415 (17) |
| C11—C12 | 1.3367 (18) | 1.347 (10) | 1.3446 (15) | 1.3438 (17) |
| C12—C13 | 1.4582 (19) | 1.449 (10) | 1.4560 (16) | 1.4575 (17) |
| C24—C27 | – | 1.472 (10) | – | – |
| C27—C28 | – | 1.345 (10) | – | – |
| C28—C29 | – | 1.421 (11) | – | – |
| C29—C30 | – | 1.347 (11) | – | – |
| C30—C31 | – | 1.439 (10) | – | – |
| C31—C32 | – | 1.370 (10) | – | – |
| C32—C33 | – | 1.446 (10) | – | – |
| | | | | |
| C5—C4—C7—C8 | −0.7 (2) | −13.2 (12) | 5.31 (18) | −3.80 (18) |
| C11—C12—C13—C18 | −7.0 (2) | −1.3 (12) | 3.65 (19) | −8.39 (19) |
| C25—C24—C27—C28 | – | 20.9 (11) | – | – |
| C31—C32—C33—C38 | – | −1.6 (11) | – | – |

All H atoms were located by geometric considerations and refined as riding on their carrier atoms.

For all compounds, data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV3067). Services for accessing these data are described at the back of the journal.

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