cis-Ethylenebis(diphenylphosphine oxide)

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The title compound, \(\text{C}_{26}\text{H}_{22}\text{O}_{2}\text{P}_{2}\), crystallizes across a twofold rotation axis. The structure is characterized by chains formed through \(\text{C} - \text{H} \cdots \text{O}\) hydrogen bonds running along the \(b\) axis, which are further supported by \(\text{C} - \text{H} \cdots \pi\) and \(\pi - \pi\) intermolecular interactions.

Comment

Complexes with phosphine oxides have been well studied (Calcagno et al., 2000; Deacon et al., 1998). The strong dipolar nature of the \(\text{P}=\text{O}\) group makes it a good hydrogen-bond acceptor, influencing the crystal packing. The structural properties of some bis-diphenylphosphine oxides are influenced by the conformation of the bridge, the orientation of the \(\text{P}=\text{O}\) dipoles and other intermolecular interactions (Calcagno et al., 2000).

Compound (I) crystallizes in the monoclinic space group \(\text{C}2\text{c}\) with one half-molecule in the asymmetric unit, the other half being generated by a crystallographic twofold rotation axis parallel to the \(b\) axis. In compound (I) (Fig. 1), the \(\text{P}=\text{O}\) bond distance is consistent with values recorded for other

![Figure 1](image-url)

The molecular structure of (I), showing the atom-numbering scheme (50% probability displacement ellipsoids). [Symmetry code: (') \(-x, y, -z + 1\).]
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Figure 2 View down the a axis, showing C—H· · ·O ribbons. Hydrogen bonds are shown as dashed lines.

Figure 3 Packing diagram, viewed down the b axis, showing C—H· · ·π and π· · ·π interactions (as dashed lines).

phosphine oxides (See et al., 1998; Bye et al., 1982). The ethylene bridge is almost planar [5.9 (2)] and the O1= P1—C13═C13 torsion angle is −33.8 (2). The angles about the P atom deviate slightly from tetrahedral geometry, with the P═O groups orientated away from each other such that the O1=P1...P1′═O1′ torsion angle is 54.96 (7)° [symmetry code: (i) −x, y, −z + 1/2]. The structure is characterized by the formation of C—H· · ·O hydrogen-bonded chains [described by a C(4) graphset (Etter et al., 1990; Bernstein et al., 1995)] which run along the b axis. These C(4) C—H· · ·O hydrogen-bonded chains (Table 1) result in rings described by the second-level R2(10) graph set (Fig. 2). Adjacent chains are linked to each other through C—H· · ·π interactions (Table 1) along the a and c axes (Fig. 3) and are further supported by π· · ·π interactions [Cg1• • • Cg2(−x, 1 − y, −z) = 3.6935 (10) Å], where Cg1 and Cg2 are the centroids of the C1—C6 and C7—C12 rings, respectively] between molecules related by a center of inversion.

Experimental

Colorless plates of the title compound were serendipitously obtained from CH2Cl2 during the attempted synthesis of some metal complexes.

Crystal data

C26H22O2P2 V = 2042.09 (6) Å³
M = 428.38 Z = 4
Monoclinic, C2/c Mo Kα radiation
a = 23.5463 (4) Å μ = 0.24 mm−1
b = 5.7654 (1) Å T = 173 (2) K
c = 17.4776 (3) Å θ = 0.36 × 0.28 × 0.10 mm
β = 120.607 (1)

Data collection

Bruker SMART CCD area-detector diffractometer 2474 independent reflections
Absorption correction: none 2175 reflections with I > 2σ(I)
12089 measured reflections Rint = 0.028

Refinement

R(F2) = 0.035 136 parameters
wR(F2) = 0.092 H-atom parameters constrained
S = 1.07 Δρmax = 0.40 e Å−3
2474 reflections Δρmin = −0.26 e Å−3

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

<table>
<thead>
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<th>D—H · · ·A</th>
<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
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<tbody>
<tr>
<td>C13—H13· · ·O1ő</td>
<td>0.95</td>
<td>2.33</td>
<td>3.2351 (16)</td>
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</tr>
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<td>C4—H4· · ·Cg2ii</td>
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<td>2.67</td>
<td>3.5514 (17)</td>
<td>154</td>
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<tr>
<td>C10—H10· · ·Cg1iii</td>
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<td>2.66</td>
<td>3.494 (2)</td>
<td>146</td>
</tr>
</tbody>
</table>

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

H atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H bond lengths of 0.93 Å and Uiso(H) = 1.2Uiso(C).

Data collection: SMART-NT (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXL97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003), ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: WinGX (Farrugia, 1999).

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References