

2-Diphenylarsino-1-(diphenylphosphino)ethane

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The title compound, C₂₆H₂₄PA₂, has inversion symmetry as a result of the orientational disorder of the molecule. The two possible positions of the As and P atoms are overlapped.

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Comment

There have been numerous X-ray structural determinations of tertiary phosphines and also tertiary arsines which are widely used as ligands in organo-transition metal chemistry. However, X-ray structure determinations of ligands containing both P and As atoms are rare. As part of our study on the substitution of transition metal–carbonyl clusters with mixed-ligand complexes, we have published several structures of triruthenium–carbonyl clusters containing mixed P/As (Shawkataly *et al.*, 1998) or P/Sb ligands (Shawkataly *et al.*, 2004). A search of the November 2004 release of the Cambridge Structural Database (Allen, 2002) revealed only 20 structures of complexes containing the above ligands.

Key indicators

Single-crystal X-ray study

T = 293 K

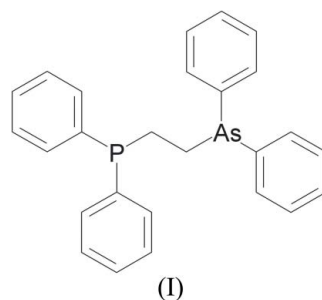
Mean $\sigma(C-C) = 0.005 \text{ \AA}$

Disorder in main residue

R factor = 0.039

wR factor = 0.096

Data-to-parameter ratio = 18.9

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, (I), is commercially available and has been widely used, though the crystal structure has not been reported.

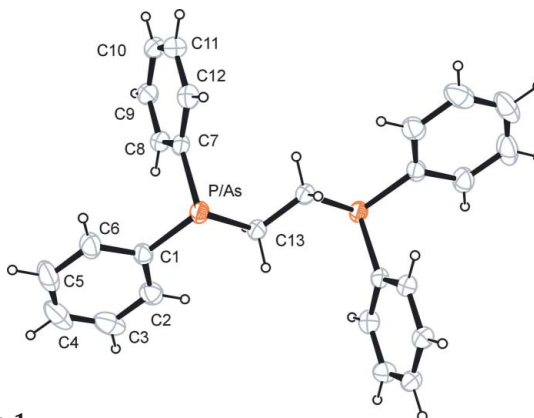


Figure 1

The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 25% probability level. Unlabeled atoms are related to labeled atoms by $(2-x, -y, 2-z)$.

The crystal structure of (I) is isomorphous with those of $\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2$ (Pelizzi & Pelizzi, 1979) and $\text{Ph}_2\text{As}(\text{CH}_2)_2\text{AsPh}_2$ (Hill *et al.*, 2001); all these compounds have a crystallographic inversion center at the mid-point of the $\text{Csp}^3\text{—Csp}^3$ bond. Positional disorder of the As and P atoms (Fig. 1). The positional disorder between the As/P atoms was also observed in $\text{Ru}_3(\text{CO})_8(\text{Ph}_2\text{AsCH}_2\text{AsPh}_2)\text{—}(\text{Ph}_2\text{PCH}_2\text{PPh}_2)$ (Shawkataly *et al.*, 1998).

Experimental

The compound was supplied by Strem Chemicals. Single crystals of (I) were obtained by slow evaporation of an ethanol solution.

Crystal data

$\text{C}_{26}\text{H}_{24}\text{AsP}$	$D_x = 1.323 \text{ Mg m}^{-3}$
$M_r = 442.34$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 40 reflections
$a = 9.1011 (6) \text{ \AA}$	$\theta = 9.9\text{--}24.3^\circ$
$b = 5.7856 (8) \text{ \AA}$	$\mu = 1.61 \text{ mm}^{-1}$
$c = 21.4502 (10) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 100.557 (5)^\circ$	Prism, colorless
$V = 1110.35 (18) \text{ \AA}^3$	$0.22 \times 0.16 \times 0.12 \text{ mm}$
$Z = 2$	

Data collection

Siemens P4 diffractometer	$R_{\text{int}} = 0.034$
$\omega/2\theta$ scans	$\theta_{\text{max}} = 27.5^\circ$
Absorption correction: ψ scan (Siemens, 1994)	$h = -1 \rightarrow 11$
$T_{\text{min}} = 0.744$, $T_{\text{max}} = 0.826$	$k = -1 \rightarrow 7$
3557 measured reflections	$l = -27 \rightarrow 27$
2520 independent reflections	3 standard reflections
1579 reflections with $I > 2\sigma(I)$	frequency: 60 min
	intensity decay: 0.2%

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.041P)^2]$
$wR(F^2) = 0.096$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2520 reflections	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
133 parameters	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

As/P—C13	1.910 (3)	As/P—C7	1.915 (2)
As/P—C1	1.912 (3)	C13—C13 ⁱ	1.520 (5)
C13—As/P—C1	100.51 (13)	C6—C1—As/P	115.8 (2)
C13—As/P—C7	98.01 (11)	C8—C7—C12	118.2 (2)
C1—As/P—C7	97.72 (10)	C8—C7—As/P	123.9 (2)
C2—C1—C6	118.7 (3)	C12—C7—As/P	117.9 (2)
C2—C1—As/P	125.3 (2)	C13 ⁱ —C13—As/P	110.3 (3)

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

The site-occupancy factors of the As and P atoms were fixed at 0.5, and the same positional and atomic displacement parameters were assumed. The methylene H atoms were located in difference density maps and their coordinates were refined [$\text{C—H} = 0.93 (3)\text{--}0.95 (3) \text{ \AA}$]. The phenyl H atoms were placed at calculated positions and refined using a riding model, with $\text{C—H} = 0.93 \text{ \AA}$. All H-atom U_{iso} parameters were fixed at $1.2U_{\text{eq}}(\text{C})$.

Data collection: XSCANS (Siemens, 1994); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS86 (Sheldrick, 1985); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX publication routines (Farrugia, 1999).

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