Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

1,2-Bis(diphenylarsino)ethane

Nicholas J. Hill, William Levason, Gillian Reid and Michael Webster*

Department of Chemistry, University of Southampton, Southampton SO17 1BJ, England

Correspondence e-mail: mw1@soton.ac.uk

Received 14 June 2001
Accepted 29 June 2001
Online 13 July 2001

The title compound, $Ph_2AsCH_2CH_2AsPh_2$ or $C_{26}H_{24}As_2$, contains discrete molecules located on an inversion centre. Changes in the C—As—C angle upon coordination are noted.

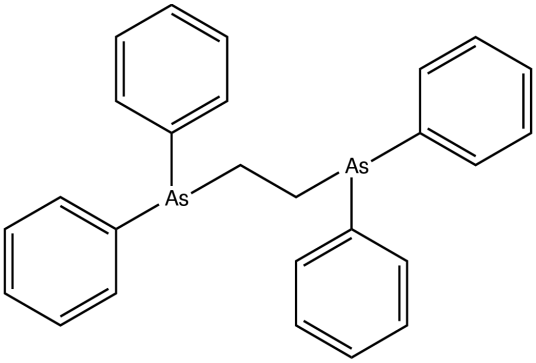
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.024
wR factor = 0.067
Data-to-parameter ratio = 15.1

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

Comment

During the course of our work on antimony(III) and bismuth(III) complexes of multidentate tertiary phosphine and arsine ligands (Genge *et al.*, 2001), 1,2-bis(diphenylarsino)ethane [(I), dpae] was isolated as colourless needles from an attempted preparation of the complex [$SbCl_3$(dpae)]. This ligand is commercially available and has been widely used although the crystal structure has not been reported.



(I)

The literature contains a number of structural reports concerning transition metal complexes of this ligand: [$Pd_3(\mu_3$-$S)_2(dpae)_3][BPh_4]_2$ (Matsumoto *et al.*, 1999), [$Ru(dpae)_2I_2$][BF_4] (Champness *et al.*, 1996), [Os(N)Cl_3(dpae)] (Lam *et al.*, 1993), [ReN$(dpae)_2$Cl][ClO_4] (Yam *et al.*, 1992), [$ReH_5(PPh_3)_2$(dpae)] (Costello *et al.*, 1991), [$Re_2Cl_4(dpae)_2$] and [$ReCl(dpae)_2]_2[Re_2Cl_8$] (Ferry *et al.*, 1989), and [$Ag(NO_3)_2$(dpae)] (Pelizzi *et al.*, 1985).

The title structure contains discrete centrosymmetric molecules (Fig. 1 and Table 1) with typical values for the C—C and As—C bond lengths. It has been noted for Ph_3M complexes (M = Sb or As) (Holmes *et al.*, 1998) that the mean C—M—C angle increases upon coordination and the same trend is observed in the compound under study. Inspection of the Cambridge Structural Database (CSD; Allen & Kennard, 1993) gave the average C—As—C bond angle in the small sample (22 observations) of dpae complexes of 103.9° (maximum 106.9°, minimum 98.9°), compared with an angle of 98.4° in the free ligand.

DOI: 10.1107/S1600536801010959

Experimental

The title compound was prepared according to the literature method of Tzschach & Lange (1962). Crystals of suitable quality for single-crystal X-ray diffraction studies were obtained by evaporation of a 1:1 *v*/*v* dichloromethane/acetonitrile solution of dpae and $SbCl_3$ during the attempted preparation of a complex.

Crystal data

$C_{26}H_{24}As_2$
$M_r = 486.29$
Monoclinic, $P2_1/n$
$a = 9.078$ (1) Å
$b = 5.761$ (2) Å
$c = 21.372$ (2) Å
$\beta = 100.341$ (8)°
$V = 1099.6$ (4) Å^3
$Z = 2$

$D_x = 1.469$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 19.2$–23.8°
$\mu = 3.05$ mm^{-1}
$T = 150$ (2) K
Needle, colourless
0.60 × 0.45 × 0.38 mm

Data collection

Rigaku AFC-7*S* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.224$, $T_{\max} = 0.314$
2061 measured reflections
1932 independent reflections
1700 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.016$
$\theta_{\max} = 25.0°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 6$
$l = -25 \rightarrow 24$
3 standard reflections every 150 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.067$
$S = 1.10$
1932 reflections
128 parameters
Only H-atom *U*'s refined

$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.007$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

As1—C8	1.959 (2)	As1—C1	1.973 (2)
As1—C2	1.962 (3)	C1—C1$^{\rm i}$	1.518 (5)
C8—As1—C2	97.95 (10)	C3—C2—As1	124.3 (2)
C8—As1—C1	97.18 (10)	C7—C2—As1	117.0 (2)
C2—As1—C1	99.93 (11)	C13—C8—C9	118.8 (2)
C1$^{\rm i}$—C1—As1	110.0 (2)	C13—C8—As1	122.43 (19)
C3—C2—C7	118.6 (3)	C9—C8—As1	118.81 (19)

Symmetry code: (i) $1-x, -y, -z$.

Data collection: *MSC*/*AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988); cell refinement: *MSC*/*AFC Diffractometer Control Software*; data reduction: *teXsan for Windows* (Molecular Structure Corporation, 1997–1999); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976).

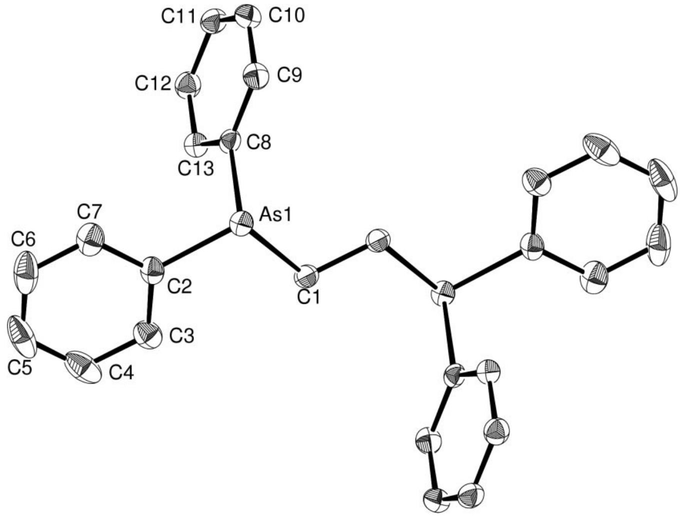


Figure 1
The molecular structure of (I) showing the atom-labelling scheme. Ellipsoids are drawn at the 40% probability level and H atoms have been omitted for clarity.

We thank EPSRC for support.

References

Allen, F. H. & Kennard, O. (1993). *Chem. Des. Autom. News*, **8**, 1, 31–37.
Champness, N. R., Levason, W., Preece, S. R., Webster, M. & Frampton, C. S. (1996). *Inorg. Chim. Acta*, **244**, 65–72.
Costello, M. T., Fanwick, P. E., Green, M. A. & Walton, R. A. (1991). *Inorg. Chem.* **30**, 861–864.
Ferry, J., Gallagher, J., Cunningham, D. & McArdle, P. (1989). *Polyhedron*, **8**, 1733–1735.
Genge, A. R. J., Hill, N. J., Levason, W. & Reid, G. (2001). *J. Chem. Soc. Dalton Trans.* pp. 1007–1012.
Holmes, N. J., Levason, W. & Webster, M. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3457–3461.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Lam, H.-W., Chin, K.-F., Che, C.-M., Wang, R.-J. & Mak, T. C. W. (1993). *Inorg. Chim. Acta*, **204**, 133–137.
Matsumoto, K., Takahashi, K., Hada, S. & Nakao, Y. (1999). *Polyhedron*, **18**, 1811–1814.
Molecular Structure Corporation (1988). *MSC*/*AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA. (Present address: MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.)
Molecular Structure Corporation (1997–1999). *teXsan for Windows*. Version 1.06. MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Pelizzi, C., Pelizzi, G. & Tarasconi, P. (1985). *J. Organomet. Chem.* **281**, 403–411.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Tzschach, A. & Lange, W. (1962). *Chem. Ber.* **95**, 1360–1366.
Yam, V. W.-W., Tam, K.-K., Cheng, M.-C., Peng, S.-M. & Wang, Y. (1992). *J. Chem. Soc. Dalton Trans.* pp. 1717–1723.