Crystal structure of *cis*-1,3-bis(phenylphosphinic acid)-2-oxapropane, $[PhP(=O)(OH)CH_2]_2O$

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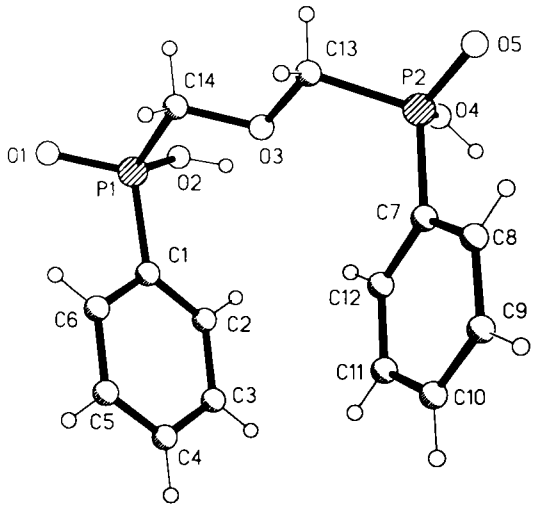

Source of material: see ref. 1; recrystallised from methanol. Bond lengths at phosphorus: P1-O1 1.482(2) Å, P1-O2 1.544(3) Å, P1–C1 1.784(3) Å, P1–C14 1.802(4) Å, P2–O5 1.486(3) Å, P2–O4 1.547(3) Å, P2–C7 1.789(4) Å, P2–C13 1.797(3) Å. The interplanar angle between the phenyl rings is 75.1(1)°. The molecules are linked into corrugated sheets parallel to the *bc* plane by short hydrogen bonds O2–H2···O5(−*x*+1, −*y*+2, *z*−1/2) with O···O 2.479(3) Å and O4–H4···O1(*x*, *y*+1, *z*) with O···O 2.514(3) Å.

$C_{14}H_{16}O_5P_2$, orthorhombic, *Pca*2$_1$ (No. 29), *a* =17.032(4) Å, *b* =8.343(2) Å, *c* =10.585(3) Å, *V* =1504.1 Å^3, *Z* =4, *R*(*F*) =0.032, $R_w(F^2)$ =0.081.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless tablet, size 0.12 x 0.40 x 0.44 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	3.07 cm^{-1}
Diffractometer:	Nicolet R3
Scan mode:	ω
$T_{measurement}$:	178 K
$2\theta_{max}$:	50.1°
$N(hkl)_{unique}$:	1406
Criterion for I_o:	Refined on F^2 for all reflections
$N(param)_{refined}$:	192
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	4*a*	0.5577	0.6882	0.1582	0.033
H(4)	4*a*	0.5256	1.1780	0.3458	0.034
H(2A)	4*a*	0.6914	0.7424	0.1770	0.041
H(3A)	4*a*	0.8219	0.8076	0.2278	0.047
H(4A)	4*a*	0.8850	0.6739	0.3926	0.048
H(5A)	4*a*	0.8215	0.4770	0.5044	0.046
H(6A)	4*a*	0.6919	0.4105	0.4578	0.038
H(8A)	4*a*	0.5775	1.1943	0.7126	0.041
H(9A)	4*a*	0.7074	1.2397	0.7746	0.045
H(10A)	4*a*	0.8102	1.1385	0.6550	0.046
H(11A)	4*a*	0.7852	0.9990	0.4697	0.047
H(12A)	4*a*	0.6565	0.9628	0.3998	0.035
H(13A)	4*a*	0.4924	0.7906	0.5811	0.033
H(13B)	4*a*	0.4264	0.8212	0.4758	0.033
H(14A)	4*a*	0.4646	0.5659	0.3885	0.031
H(14B)	4*a*	0.5364	0.5467	0.4856	0.031

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P(1)	4*a*	0.58043(5)	0.51145(9)	0.2787(1)	0.0243(4)	0.0180(4)	0.0203(4)	−0.0007(3)	−0.0001(4)	−0.0008(4)
P(2)	4*a*	0.50396(5)	1.0486(1)	0.4999(1)	0.0249(5)	0.0209(4)	0.0232(4)	0.0011(4)	0.0009(4)	−0.0021(4)
O(1)	4*a*	0.5721(1)	0.3346(3)	0.2756(3)	0.036(1)	0.020(1)	0.033(1)	−0.003(1)	−0.001(1)	−0.001(1)
O(2)	4*a*	0.5543(2)	0.5880(3)	0.1528(2)	0.033(1)	0.025(1)	0.024(1)	0.000(1)	−0.006(1)	−0.001(1)
O(3)	4*a*	0.5304(1)	0.7610(3)	0.4049(2)	0.029(1)	0.018(1)	0.030(1)	−0.002(1)	0.010(1)	−0.001(1)
O(4)	4*a*	0.4973(1)	1.0975(3)	0.3594(2)	0.033(1)	0.025(1)	0.028(1)	−0.007(1)	−0.006(1)	0.000(1)
O(5)	4*a*	0.4477(1)	1.1265(3)	0.5879(2)	0.030(1)	0.028(1)	0.036(2)	0.003(1)	0.004(1)	−0.007(1)
C(1)	4*a*	0.6791(2)	0.5694(4)	0.3117(3)	0.024(2)	0.021(2)	0.023(2)	0.002(1)	−0.001(1)	−0.006(1)
C(2)	4*a*	0.7176(2)	0.6881(5)	0.2437(4)	0.028(2)	0.028(2)	0.041(2)	0.001(2)	−0.002(2)	0.001(2)
C(3)	4*a*	0.7949(2)	0.7269(5)	0.2740(5)	0.030(2)	0.032(2)	0.057(3)	−0.003(2)	0.005(2)	0.001(2)
C(4)	4*a*	0.8324(2)	0.6470(5)	0.3718(5)	0.028(2)	0.034(2)	0.065(3)	0.003(2)	−0.012(2)	−0.017(2)
C(5)	4*a*	0.7948(2)	0.5311(5)	0.4381(4)	0.034(2)	0.038(2)	0.040(2)	0.007(2)	−0.012(2)	−0.009(2)

Table 3. (Continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(6)	4*a*	0.7181(2)	0.4910(4)	0.4102(4)	0.033(2)	0.031(2)	0.025(2)	0.005(1)	–0.005(2)	–0.004(2)
C(7)	4*a*	0.6036(2)	1.0772(4)	0.5481(3)	0.027(2)	0.022(2)	0.023(2)	–0.001(1)	–0.001(2)	0.001(1)
C(8)	4*a*	0.6195(2)	1.1570(4)	0.6614(4)	0.031(2)	0.037(2)	0.028(2)	0.003(2)	–0.002(2)	–0.005(2)
C(9)	4*a*	0.6967(2)	1.1818(5)	0.6993(4)	0.043(2)	0.047(2)	0.026(2)	–0.005(2)	–0.007(2)	–0.005(2)
C(10)	4*a*	0.7576(2)	1.1226(4)	0.6280(4)	0.028(2)	0.040(2)	0.040(2)	–0.008(2)	–0.008(2)	0.009(2)
C(11)	4*a*	0.7428(3)	1.0406(4)	0.5178(5)	0.031(2)	0.039(2)	0.040(2)	–0.001(2)	0.005(2)	0.003(2)
C(12)	4*a*	0.6663(2)	1.0182(4)	0.4766(4)	0.027(2)	0.033(2)	0.027(2)	–0.001(1)	–0.001(2)	–0.004(2)
C(13)	4*a*	0.4824(2)	0.8378(4)	0.4968(4)	0.032(2)	0.021(2)	0.023(2)	0.000(1)	0.006(2)	–0.004(2)
C(14)	4*a*	0.5205(2)	0.5928(4)	0.4034(3)	0.033(2)	0.020(2)	0.026(2)	–0.003(1)	0.006(2)	–0.002(2)

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