Crystal structure of 1-hydroxy-1-phenyl-methylidene-1,1-bisphosphonic acid tetrabenzyl ester, $C_{35}H_{34}O_7P_2$

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Source of material: The compound was prepared as described in reference 1 and crystallized from chloroform/ether (5:1) by slow evaporation at room temperature

The molecules are linked together by hydrogen bonds $O10 \cdots O21 = 2.669(4)$ Å or $H10 \cdots O21 = 1.936(3)$ Å. Cohesion of the crystal is permitted by the aromatic cycles that form staggered layers in several directions.

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

Crystal:	colorless plate, size 0.2 x 0.25 x 0.3 mm
Wavelength:	Cu K_{α} radiation (1.54180 Å)
μ :	16.43 cm ⁻¹
Diffractometer:	Philips PW1100
Scan mode:	$\theta/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	126°
$N(hkl)_{\text{unique}}$:	3183
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	397
Programs:	SHELXS-86, SHELXL-93

$C_{35}H_{34}O_7P_2$, monoclinic, $P12_1/c1$ (No. 14), $a = 14.427(2)$ Å, $b = 27.941(2)$ Å, $c = 8.246(2)$ Å, $\beta = 107.0(1)^\circ$, $V = 3178.8$ Å³, $Z = 4$, $R(F) = 0.062$, $R_w(F^2) = 0.263$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(10)	4e	0.0408	-0.0061	0.6955	0.05
H(2)	4e	0.3726	-0.0039	0.8493	0.05
H(3)	4e	0.4868	-0.0495	1.0592	0.05
H(4)	4e	0.4375	-0.1057	1.2278	0.05
H(5)	4e	0.2683	-0.1167	1.1951	0.05
H(6)	4e	0.1503	-0.0706	0.9853	0.05
H(12A)	4e	0.3781	0.1048	1.0640	0.05
H(12B)	4e	0.2729	0.1237	1.0425	0.05
H(122)	4e	0.1986	0.1728	0.7603	0.05
H(123)	4e	0.2310	0.2437	0.6307	0.05
H(124)	4e	0.3909	0.2718	0.6912	0.05
H(125)	4e	0.5211	0.2294	0.8733	0.05
H(126)	4e	0.4893	0.1570	1.0080	0.05
H(13A)	4e	0.0495	0.0396	1.1011	0.05
H(13B)	4e	0.0113	0.0619	0.9188	0.05
H(132)	4e	0.0832	0.0872	1.3482	0.05
H(133)	4e	0.0807	0.1626	1.4714	0.05
H(134)	4e	0.0456	0.2324	1.3003	0.05
H(135)	4e	0.0154	0.2260	1.0008	0.05
H(136)	4e	0.0363	0.1498	0.8767	0.05
H(22A)	4e	0.2487	0.0205	0.2952	0.05
H(22B)	4e	0.3372	-0.0138	0.3708	0.05
H(222)	4e	0.2863	0.1061	0.4799	0.05
H(223)	4e	0.3924	0.1726	0.4940	0.05
H(224)	4e	0.5423	0.1621	0.4335	0.05
H(225)	4e	0.5871	0.0849	0.3549	0.05
H(226)	4e	0.4786	0.0190	0.3348	0.05
H(23A)	4e	0.0967	-0.1066	0.4130	0.05
H(23B)	4e	0.1053	-0.1041	0.6072	0.05
H(232)	4e	0.0872	-0.1888	0.3552	0.05
H(233)	4e	0.1630	-0.2654	0.4032	0.05
H(234)	4e	0.3032	-0.2777	0.6308	0.05
H(235)	4e	0.3736	-0.2137	0.8119	0.05
H(236)	4e	0.3018	-0.1368	0.7692	0.05

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P(1)	4e	0.17277(5)	0.05866(4)	0.8219(1)	0.0401(5)	0.048(1)	0.041(1)	-0.0004(3)	0.0109(4)	0.0050(5)
P(2)	4e	0.18469(5)	-0.01639(4)	0.5506(1)	0.0334(5)	0.056(1)	0.035(1)	-0.0034(3)	0.0070(4)	0.0007(5)
O(11)	4e	0.0997(2)	0.0854(1)	0.6934(3)	0.059(1)	0.056(2)	0.047(2)	0.011(1)	0.009(1)	0.008(2)
O(12)	4e	0.2794(2)	0.0765(1)	0.8628(4)	0.051(1)	0.050(2)	0.059(2)	-0.011(1)	0.023(1)	-0.008(2)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(13)	4e	0.1564(2)	0.0569(1)	1.0015(3)	0.052(1)	0.063(2)	0.035(2)	0.003(1)	0.020(1)	0.001(1)
O(21)	4e	0.0958(1)	-0.0032(1)	0.4181(3)	0.041(1)	0.069(2)	0.038(2)	0.003(1)	0.004(1)	0.003(1)
O(22)	4e	0.2782(2)	0.0111(1)	0.5461(3)	0.044(1)	0.070(2)	0.036(2)	-0.008(1)	0.013(1)	0.003(1)
O(23)	4e	0.2141(1)	-0.07009(9)	0.5484(3)	0.044(1)	0.052(2)	0.055(2)	-0.003(1)	0.013(1)	-0.012(1)
C(10)	4e	0.1768(2)	-0.0046(1)	0.7640(5)	0.036(1)	0.054(3)	0.033(3)	-0.003(1)	0.012(1)	0.001(2)
O(10)	4e	0.0830(1)	-0.02238(9)	0.7632(3)	0.031(1)	0.062(2)	0.054(2)	-0.0051(9)	0.012(1)	0.012(1)
C(1)	4e	0.2510(2)	-0.0334(1)	0.9005(5)	0.042(2)	0.045(3)	0.028(3)	0.004(1)	0.003(1)	-0.004(2)
C(2)	4e	0.3495(2)	-0.0275(2)	0.9218(5)	0.043(2)	0.062(3)	0.050(3)	0.002(1)	0.007(2)	0.004(2)
C(3)	4e	0.4153(3)	-0.0543(2)	1.0432(7)	0.047(2)	0.093(4)	0.054(3)	0.021(2)	-0.002(2)	-0.001(3)
C(4)	4e	0.3875(3)	-0.0864(2)	1.1411(6)	0.073(2)	0.090(4)	0.039(3)	0.031(2)	0.002(2)	0.010(3)
C(5)	4e	0.2902(3)	-0.0929(2)	1.1219(7)	0.085(3)	0.077(4)	0.061(4)	0.018(2)	0.015(2)	0.021(3)
C(6)	4e	0.2217(3)	-0.0660(2)	0.9999(6)	0.058(2)	0.063(3)	0.044(3)	0.007(2)	0.015(2)	0.009(2)
C(12)	4e	0.3190(3)	0.1156(2)	0.9817(6)	0.072(2)	0.061(4)	0.054(3)	-0.019(2)	0.003(2)	0.003(3)
C(121)	4e	0.3398(3)	0.1582(2)	0.8962(6)	0.064(2)	0.047(3)	0.049(3)	-0.011(2)	0.020(2)	-0.009(2)
C(122)	4e	0.2677(3)	0.1842(2)	0.7879(7)	0.073(2)	0.073(4)	0.085(4)	0.005(2)	0.004(2)	0.022(3)
C(123)	4e	0.2858(5)	0.2255(3)	0.7114(9)	0.122(5)	0.101(6)	0.103(5)	0.035(4)	0.017(4)	0.033(4)
C(124)	4e	0.3776(6)	0.2412(2)	0.7457(9)	0.157(6)	0.056(4)	0.098(5)	-0.013(4)	0.035(4)	0.012(4)
C(125)	4e	0.4526(5)	0.2172(3)	0.8508(9)	0.115(4)	0.105(5)	0.098(5)	-0.052(4)	0.046(4)	-0.024(4)
C(126)	4e	0.4339(3)	0.1752(2)	0.9283(6)	0.072(2)	0.077(4)	0.068(4)	-0.018(2)	0.026(2)	-0.011(3)
C(13)	4e	0.0612(3)	0.0643(2)	1.0268(6)	0.052(2)	0.077(4)	0.061(4)	-0.001(2)	0.029(2)	-0.001(3)
C(131)	4e	0.0563(2)	0.1116(2)	1.1019(7)	0.052(2)	0.066(4)	0.048(4)	0.003(2)	0.017(2)	-0.001(3)
C(132)	4e	0.0705(3)	0.1166(2)	1.2737(8)	0.063(2)	0.054(4)	0.055(5)	0.003(2)	0.018(2)	-0.009(3)
C(133)	4e	0.0680(4)	0.1599(3)	1.3447(8)	0.122(4)	0.084(6)	0.052(4)	0.003(3)	0.030(3)	0.003(5)
C(134)	4e	0.0485(7)	0.2001(3)	1.247(1)	0.226(8)	0.093(7)	0.091(7)	0.023(5)	0.093(6)	-0.025(6)
C(135)	4e	0.0329(8)	0.1966(3)	1.075(1)	0.29(1)	0.058(6)	0.142(9)	0.072(5)	0.131(7)	0.049(5)
C(136)	4e	0.0412(5)	0.1522(3)	1.0011(7)	0.147(5)	0.094(6)	0.054(4)	0.035(3)	0.053(3)	0.027(4)
C(22)	4e	0.3058(3)	0.0154(2)	0.3907(6)	0.065(2)	0.077(4)	0.034(3)	-0.006(2)	0.025(2)	-0.002(2)
C(221)	4e	0.3739(2)	0.0568(2)	0.4084(5)	0.052(2)	0.057(3)	0.025(3)	-0.001(2)	0.014(1)	0.007(2)
C(222)	4e	0.3497(3)	0.1014(2)	0.4530(6)	0.061(2)	0.068(4)	0.062(3)	-0.005(2)	0.028(2)	0.000(3)
C(223)	4e	0.4112(4)	0.1400(2)	0.4616(6)	0.101(3)	0.065(4)	0.056(4)	0.008(2)	0.024(2)	-0.009(3)
C(224)	4e	0.4975(3)	0.1339(2)	0.4262(6)	0.075(2)	0.074(4)	0.055(3)	-0.024(2)	0.020(2)	0.015(3)
C(225)	4e	0.5234(2)	0.0895(2)	0.3806(6)	0.051(2)	0.084(4)	0.056(3)	-0.010(2)	0.019(2)	0.012(3)
C(226)	4e	0.4607(2)	0.0514(2)	0.3705(5)	0.058(2)	0.066(3)	0.039(3)	0.009(2)	0.018(2)	0.012(2)
C(23)	4e	0.1417(3)	-0.1082(2)	0.5262(8)	0.044(2)	0.069(4)	0.131(5)	-0.010(2)	0.011(2)	-0.027(3)
C(231)	4e	0.1895(2)	-0.1546(2)	0.5513(6)	0.053(2)	0.056(4)	0.074(4)	-0.001(2)	0.019(2)	-0.016(2)
C(232)	4e	0.1489(4)	-0.1932(2)	0.4509(9)	0.089(3)	0.083(5)	0.122(5)	0.000(3)	0.000(3)	-0.036(4)
C(233)	4e	0.1922(4)	-0.2378(2)	0.480(1)	0.105(4)	0.067(4)	0.144(6)	0.000(3)	0.026(4)	-0.034(4)
C(234)	4e	0.2727(4)	-0.2448(2)	0.611(1)	0.093(4)	0.054(4)	0.182(7)	0.013(3)	0.056(4)	0.017(4)
C(235)	4e	0.3131(4)	-0.2082(3)	0.7146(8)	0.099(3)	0.074(5)	0.112(5)	0.014(3)	0.032(3)	0.037(4)
C(236)	4e	0.2722(3)	-0.1636(2)	0.6886(7)	0.076(3)	0.071(4)	0.080(4)	-0.007(2)	0.023(2)	0.004(3)

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References

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