CRYSTAL STRUCTURE OF 1,1,2,2-TETRAPHENYL-1,2-DIHYDROXYDISILANE, $[\text{Ph}_2(\text{OH})\text{Si}]_2$

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Figure 1. Molecular structure (30 % probability ellipsoids) of $[\text{Ph}_2(\text{OH})\text{Si}]_2$. Symmetry transformations used to generate equivalent atoms: $a = -x, -y, 1 - z$. Selected bond distances (Å) and angles (°), and ranges of bond distances (Å) and angles (°), respectively: O(1)-O(3a) 2.676(3), O(1)-O(5a) 2.758(2), O(2)-O(3) 2.796(3), O(2)-O(2a) 2.756(4), O(4)-O(5) 2.706(3), O(4)-O(6b) 2.737(3), O(6)-O(6b) 2.788(4), O(1)-Si(1)-Si(2)-O(2) 68.5(1), O(3)-Si(3)-Si(4)-O(4) -70.4(1), O(5)-Si(5)-Si(6)-O(6) -67.5(1); Si-Si 2.360(1)-2.379(1), Si-O 1.658(2)-1.666(2), C-Si-C 104.03(9)-117.69(9), O-Si-C 106.7(1)-110.3(1), O-Si-Si 108.80(9)-114.47(8).

COMMENT

In context with our interest on the chemistry of stannasiloxanes [1] we report here the crystal structure of the title compound [2] which is the only third representative of a 1,2-disilanol [3, 4] being characterized in the solid state. The unit cell contains three crystallographically independent molecules which differ slightly in their geometric parameters. The three independent molecules are linked by intermolecular O-H...O hydrogen bridges among each other and to their symmetry-related molecules to give an infinite chain.

Table 1. Crystal data for $[\text{Ph}_2(\text{OH})\text{Si}]_2$

Formula	$\text{C}_{24}\text{H}_{22}\text{O}_2\text{Si}_2$	Formula weight	398.60
Cryst syst	triclinic	Crystal size, mm	0.20 x 0.20 x 0.20
Space group	P-1	a, Å	13.365(1)
b, Å	14.700(1)	c, Å	19.507(1)
α , °	103.654(1)	β , °	101.219(1)
γ , °	113.701(1)	V, Å ³	3224.6(4)
Temperature, K	291(1)	Z	6
μ (Mo-K α), mm ⁻¹	0.181	Diffractometer	Nonius KappaCCD
D_{calcd} , g cm ⁻³	1.232	F(000)	1260
θ_{max} , °	25.0	Reflns meas.	41295
Reflns unique, R_{int}	10574, 0.054	Reflns with $I > 2\sigma(I)$	4588
Weighting scheme	$1/[\sigma^2(F_o^2) + (0.0259P)^2]$	R(F) ($I > 2\sigma(I)$)	0.047
Programs used	SHELXS97[5] SHELXL97[6] SHELXTL[7]	$R_w(F^2)$ (all data)	0.083
		ρ , e Å ⁻³	0.22 and -0.21
		Deposition number	CCDC 183142

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