

Palanquin-like Cu_4Na_4 silsesquioxane. Synthesis (via oxidation of 1,1-bis(diphenylphosphino)methane), structure and catalytic activity in alkane or alcohol oxidation with peroxides

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General Considerations

All reagents were purchased from the usual suppliers and used without further purification. IR spectrum for **1** was recorded on Shimadzu IR Prestige21 FTIR spectrometer in KBr pellets. Set of signals: 1200 cm^{-1} ($\nu\text{ P=O}$); 1140 cm^{-1} ($\nu\text{ P=O}$), 1120 cm^{-1} ($\nu\text{ Ph-Si}$), $940\text{--}1100\text{ cm}^{-1}$ ($\nu\text{ asSi-O}$, $\nu\text{ asSi-O-Si}$), 900 cm^{-1} ($\nu\text{ asSi-O}$ in Si-O-M fragment), $720\text{--}680\text{ cm}^{-1}$ ($\sigma\text{ C-H}$ of mono-substituted phenyl group)

Synthesis of **1**:

1 g (4.16 mmol) of $\text{PhSi}(\text{OEt})_3$ and 0.17 g (4.16 mmol) of NaOH were heated at reflux in 55 ml of ethanol for 2 h. Then 0.19 g (2.08 mmol) of CuCl_2 was added and resulted blue-colored mixture was stirred without heating for 1.5 h. Afterwards 0.27 g (0.70 mmol) of dppm dissolved in 30 ml of toluene was added at once and resulted mixture was stirred for 2 h. Solution was filtered from precipitate. Crystallization of filtrate (in the presence of a trace of air) gave in 3 weeks a crystalline material, several single crystals were used for X-ray

diffraction analysis ($\mathbf{1} \cdot 4\text{EtOH} \cdot 4\text{C}_7\text{H}_8$), see below for details). Analysis of complex **1** – calcd. for $[(\text{PhSiO}_{1.5})_{12}(\text{CuO})_4(\text{NaO}_{0.5})_4[(\text{C}_{25}\text{H}_{22}\text{O}_2\text{P}_2)_2]_2]$ Si, 11.93; Cu, 9.00; Na, 3.25; P, 4.39. Found (for vacuum dried sample): Si, 11.87; Cu, 8.95; Na, 3.21; P, 4.34. Yield 0.21 g (22 %).

X-ray Crystallographic Data Collection and Refinement of the Structure

Experimental part

The single-crystal X-ray diffraction data for **1** were collected on the ‘Belok’ beamline of the Kurchatov Synchrotron Radiation Source (National Research Center ‘Kurchatov Institute’, Moscow, Russian Federation) using a Rayonix SX165 CCD detector at $\lambda = 0.96990 \text{ \AA}$. A total of 720 images for two different orientations of the crystal were collected using an oscillation range of 1.0° and φ scanning mode. The data were indexed and integrated using the utility iMOSFLM from the CCP4 program suite [1] and then scaled and corrected for absorption using the Scala program [2]. For details, see Table 1. The structure was determined by direct methods and refined by full-matrix least square technique on F^2 in anisotropic approximation for non-hydrogen atoms. The two phenyl substituents and two ethanol molecules were disordered over two sites each with the occupancies of 0.50:0.50, 0.50:0.50, and 0.75:0.25, 0.75:0.25, respectively. The crystal of **1** contained the two toluene solvate molecules in the asymmetric unit, one of them was disordered over two sites with the equal occupancies. The hydrogen atoms of the OH-groups of ethanol molecules were localized in the difference-Fourier maps and included into the refinement within the riding model with fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$]. The other hydrogen atoms were placed in calculated positions and refined within the riding model with fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl groups and $1.2U_{\text{eq}}(\text{C})$ for the other groups]. All calculations were carried out using the SHELXTL program suite [3].

Crystallographic data for **1** have been deposited with the Cambridge Crystallographic Data Center, CCDC 1883934. The supplementary crystallographic data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal data and structure refinement for **1**.

Identification code	Cu8341	
Empirical formula	C158 H160 Cu4 Na4 O32 P4 Si12	
Formula weight	3377.99	
Temperature	100(2) K	
Wavelength	0.96990 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	a = 16.458(3) Å	$\alpha = 90^\circ$
	b = 24.128(5) Å	$\beta = 99.55(3)^\circ$
	c = 21.698(4) Å	$\gamma = 90^\circ$
Volume	8497(3) Å ³	
Z	2	
Density (calculated)	1.320 Mg/m ³	
Absorption coefficient	1.610 mm ⁻¹	
F(000)	3504	
Crystal size	0.20 × 0.12 × 0.10 mm ³	
Theta range for data collection	3.426 to 38.527 °	
Index ranges	-21 ≤ h ≤ 21, -29 ≤ k ≤ 29, -25 ≤ l ≤ 25	
Reflections collected	95692	
Independent reflections	17712 [R(int) = 0.0865]	
Completeness to theta = 35.587 °	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.840 and 0.740	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	17712 / 123 / 944	
Goodness-of-fit on F ²	1.054	
Final R indices [for 12971 rflns with I > 2σ(I)]	R1 = 0.0844, wR2 = 0.1689	
R indices (all data)	R1 = 0.1088, wR2 = 0.1875	
Extinction coefficient	0.00191(11)	
Largest diff. peak and hole	1.042 and -1.193 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Cu(1)	4103(1)	4411(1)	5393(1)	30(1)
Cu(2)	6370(1)	4595(1)	5422(1)	30(1)
P(1)	6883(1)	2812(1)	7311(1)	34(1)
P(2)	8754(1)	2954(1)	7248(1)	39(1)
Si(1)	4663(1)	4723(1)	6847(1)	30(1)
Si(2)	3603(1)	5514(1)	6070(1)	31(1)
Si(3)	3791(1)	6548(1)	5348(1)	33(1)
Si(4)	5673(1)	6703(1)	5382(1)	34(1)
Si(5)	6677(1)	5798(1)	6048(1)	34(1)
Si(6)	6516(1)	4851(1)	6896(1)	30(1)
Na(1)	5533(1)	3657(1)	6150(1)	35(1)
Na(2)	7444(1)	3721(1)	6176(1)	37(1)
O(1)	4311(2)	5352(1)	6663(2)	32(1)
O(2)	3624(2)	6178(1)	5952(2)	35(1)
O(3)	4728(2)	6792(2)	5508(2)	40(1)
O(4)	6214(2)	6396(1)	5996(2)	36(1)
O(5)	6637(2)	5510(1)	6720(2)	34(1)
O(6)	5637(2)	4792(1)	7151(2)	34(1)
O(7)	4543(2)	4323(1)	6253(2)	35(1)
O(8)	3781(2)	5197(2)	5454(2)	37(1)
O(9)	3639(2)	6203(2)	4704(2)	36(1)
O(10)	5704(2)	6364(2)	4753(2)	37(1)
O(11)	6238(2)	5404(2)	5487(2)	39(1)
O(12)	6583(2)	4464(1)	6309(2)	35(1)
O(13)	6645(2)	3223(2)	6794(2)	37(1)
O(14)	8556(3)	3254(2)	6662(2)	60(1)
O(15)	4516(3)	2955(2)	6284(2)	60(1)
O(16)	8244(4)	4445(3)	5771(3)	117(2)
C(1)	4122(3)	4453(2)	7482(3)	35(1)
C(2)	3653(4)	3972(2)	7404(3)	45(1)
C(3)	3227(4)	3781(3)	7864(3)	55(2)
C(4)	3277(4)	4064(3)	8422(3)	49(2)
C(5)	3747(4)	4544(3)	8518(3)	47(2)
C(6)	4160(4)	4733(2)	8051(3)	44(1)
C(7)	2569(2)	5305(2)	6280(2)	38(1)

C(8)	2323(4)	4753(2)	6190(3)	51(3)
C(9)	1586(4)	4576(2)	6368(4)	82(6)
C(8')	1944(4)	5090(3)	5832(2)	76(5)
C(9')	1207(4)	4916(4)	6010(3)	97(6)
C(10)	1109(3)	4960(3)	6635(3)	85(3)
C(11)	1389(4)	5507(3)	6714(4)	78(5)
C(12)	2113(4)	5684(2)	6539(4)	49(3)
C(11')	1733(4)	5172(4)	7082(2)	82(5)
C(12')	2470(4)	5347(4)	6903(2)	65(4)
C(13)	3109(8)	7167(4)	5307(6)	57(1)
C(14)	2688(6)	7321(4)	5787(5)	57(1)
C(15)	2255(6)	7821(4)	5752(4)	57(1)
C(16)	2245(6)	8166(3)	5235(5)	57(1)
C(17)	2666(8)	8013(4)	4754(5)	57(1)
C(18)	3099(9)	7514(5)	4790(5)	57(1)
C(13')	3069(7)	7181(4)	5322(6)	57(1)
C(14')	2517(7)	7207(3)	5746(5)	57(1)
C(15')	1967(6)	7650(4)	5723(5)	57(1)
C(16')	1967(6)	8066(3)	5277(5)	57(1)
C(17')	2518(8)	8040(4)	4854(5)	57(1)
C(18')	3068(8)	7598(5)	4876(6)	57(1)
C(19)	6125(4)	7412(2)	5329(2)	37(1)
C(20)	5646(4)	7848(2)	5032(3)	46(1)
C(21)	5991(5)	8365(3)	4941(3)	56(2)
C(22)	6814(5)	8458(3)	5146(3)	55(2)
C(23)	7306(4)	8036(3)	5454(3)	55(2)
C(24)	6963(4)	7519(2)	5538(3)	45(1)
C(25)	7800(4)	5894(2)	5992(3)	42(1)
C(26)	8048(5)	6061(3)	5430(3)	57(2)
C(27)	8873(5)	6107(4)	5386(4)	73(2)
C(28)	9474(5)	5991(4)	5892(4)	70(2)
C(29)	9251(4)	5836(3)	6448(4)	63(2)
C(30)	8422(4)	5786(3)	6501(3)	48(2)
C(31)	7318(3)	4677(2)	7594(3)	34(1)
C(32)	8141(3)	4589(2)	7546(3)	38(1)
C(33)	8728(4)	4476(2)	8076(3)	45(1)
C(34)	8495(4)	4444(2)	8659(3)	47(2)
C(35)	7681(4)	4530(3)	8717(3)	48(2)
C(36)	7099(4)	4648(2)	8195(2)	37(1)
C(37)	6243(3)	2870(2)	7907(3)	37(1)

C(38)	6102(4)	2426(3)	8290(3)	51(2)
C(39)	5606(5)	2491(3)	8743(3)	60(2)
C(40)	5250(4)	3007(3)	8825(3)	59(2)
C(41)	5380(4)	3449(3)	8450(3)	52(2)
C(42)	5877(4)	3382(2)	7988(3)	42(1)
C(43)	6794(3)	2106(2)	7031(3)	38(1)
C(44)	6172(5)	1992(3)	6526(3)	62(2)
C(45)	6087(6)	1464(3)	6283(4)	76(3)
C(46)	6599(5)	1042(3)	6532(3)	59(2)
C(47)	7190(4)	1143(2)	7036(3)	47(2)
C(48)	7280(4)	1671(2)	7295(3)	43(1)
C(49)	7927(3)	2928(2)	7728(3)	38(1)
C(50)	9626(4)	3252(3)	7754(3)	43(1)
C(51)	9788(4)	3176(3)	8404(3)	58(2)
C(52)	10483(5)	3404(4)	8757(4)	75(2)
C(53)	11017(5)	3722(4)	8472(4)	72(2)
C(54)	10874(4)	3805(3)	7830(4)	62(2)
C(55)	10178(4)	3566(3)	7475(3)	52(2)
C(56)	9032(4)	2246(3)	7126(3)	44(1)
C(57)	8876(5)	2035(3)	6524(3)	62(2)
C(58)	9038(6)	1477(3)	6417(4)	83(3)
C(59)	9358(6)	1138(3)	6909(4)	78(2)
C(60)	9539(5)	1342(3)	7513(4)	62(2)
C(61)	9374(4)	1899(3)	7624(3)	49(2)
C(62)	3867(7)	2625(4)	6449(4)	92(3)
C(63)	4100(7)	2367(4)	7087(4)	97(3)
C(64)	8981(6)	4298(5)	5542(7)	117(2)
C(65)	8901(8)	3738(4)	5214(7)	117(2)
C(64')	8419(16)	4510(20)	5151(5)	117(2)
C(65')	9309(18)	4672(19)	5146(15)	117(2)
C(66)	1121(4)	5338(2)	8892(3)	126(2)
C(67)	1960(4)	5226(3)	9061(3)	126(2)
C(68)	2230(4)	4865(3)	9555(3)	126(2)
C(69)	1662(5)	4617(3)	9878(3)	126(2)
C(70)	824(5)	4729(3)	9710(3)	126(2)
C(71)	553(4)	5090(3)	9215(3)	126(2)
C(72)	830(6)	5725(3)	8363(3)	126(2)
C(73)	3421(5)	7457(4)	8432(5)	115(3)
C(74)	3511(6)	7324(5)	7822(5)	115(3)
C(75)	3419(6)	6776(5)	7617(6)	115(3)

C(76)	3237(7)	6362(4)	8022(7)	115(3)
C(77)	3147(8)	6496(4)	8633(7)	115(3)
C(78)	3239(7)	7044(5)	8838(5)	115(3)
C(79)	3519(8)	8044(4)	8655(8)	115(3)
C(80)	4547(6)	5311(4)	10062(4)	82(3)
C(81)	5089(6)	5421(5)	9647(5)	82(3)
C(82)	5644(7)	5014(6)	9524(5)	82(3)
C(83)	5655(8)	4499(5)	9816(6)	82(3)
C(84)	5113(8)	4389(4)	10231(6)	82(3)
C(85)	4558(7)	4796(4)	10355(5)	82(3)
C(86)	3953(7)	5747(5)	10194(6)	82(3)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Cu(1)-O(7)	1.898(4)	Si(5)-C(25)	1.886(7)
Cu(1)-O(10)#1	1.932(4)	Si(6)-O(12)	1.599(4)
Cu(1)-O(11)#1	1.951(4)	Si(6)-O(6)	1.638(4)
Cu(1)-O(8)	1.980(4)	Si(6)-O(5)	1.654(4)
Cu(1)-Cu(2)#1	3.0057(10)	Si(6)-C(31)	1.883(6)
Cu(2)-O(12)	1.924(4)	Na(1)-O(7)	2.326(4)
Cu(2)-O(8)#1	1.941(4)	Na(1)-O(13)	2.356(4)
Cu(2)-O(9)#1	1.945(4)	Na(1)-O(15)	2.433(5)
Cu(2)-O(11)	1.971(4)	Na(1)-O(9)#1	2.498(4)
Cu(2)-Cu(1)#1	3.0057(10)	Na(1)-O(10)#1	2.582(4)
P(1)-O(13)	1.500(4)	Na(1)-O(12)	2.588(4)
P(1)-C(37)	1.804(6)	Na(2)-O(14)	2.255(5)
P(1)-C(43)	1.807(6)	Na(2)-O(12)	2.332(4)
P(1)-C(49)	1.826(6)	Na(2)-O(13)	2.358(4)
P(2)-O(14)	1.454(5)	Na(2)-O(9)#1	2.393(4)
P(2)-C(56)	1.801(6)	Na(2)-O(16)	2.437(7)
P(2)-C(50)	1.805(6)	O(8)-Cu(2)#1	1.941(4)
P(2)-C(49)	1.846(6)	O(9)-Cu(2)#1	1.945(4)
Si(1)-O(7)	1.596(4)	O(9)-Na(2)#1	2.393(4)
Si(1)-O(6)	1.637(4)	O(9)-Na(1)#1	2.498(4)
Si(1)-O(1)	1.649(4)	O(10)-Cu(1)#1	1.932(4)
Si(1)-C(1)	1.877(6)	O(10)-Na(1)#1	2.582(4)
Si(2)-O(8)	1.609(4)	O(11)-Cu(1)#1	1.951(4)
Si(2)-O(2)	1.624(4)	O(15)-C(62)	1.424(10)
Si(2)-O(1)	1.634(4)	O(15)-H(15O)	0.9091
Si(2)-C(7)	1.901(4)	O(16)-C(64')	1.429(3)
Si(3)-O(9)	1.609(4)	O(16)-C(64)	1.430(3)
Si(3)-O(3)	1.635(4)	O(16)-H(16O)	0.9001
Si(3)-O(2)	1.647(4)	C(1)-C(2)	1.388(8)
Si(3)-C(13)	1.861(8)	C(1)-C(6)	1.399(8)
Si(3)-C(13')	1.930(8)	C(2)-C(3)	1.391(9)
Si(4)-O(10)	1.598(4)	C(2)-H(2)	0.9500
Si(4)-O(3)	1.636(4)	C(3)-C(4)	1.381(9)
Si(4)-O(4)	1.650(4)	C(3)-H(3)	0.9500
Si(4)-C(19)	1.878(6)	C(4)-C(5)	1.389(9)
Si(5)-O(11)	1.618(4)	C(4)-H(4)	0.9500
Si(5)-O(5)	1.625(4)	C(5)-C(6)	1.388(8)
Si(5)-O(4)	1.629(4)	C(5)-H(5)	0.9500

C(6)-H(6)	0.9500	C(16')-H(16B)	0.9500
C(7)-C(12)	1.364(4)	C(17')-C(18')	1.395(3)
C(7)-C(12')	1.392(3)	C(17')-H(17B)	0.9500
C(7)-C(8')	1.393(3)	C(18')-H(18B)	0.9500
C(7)-C(8)	1.395(3)	C(19)-C(24)	1.403(8)
C(8)-C(9)	1.399(3)	C(19)-C(20)	1.405(8)
C(8)-H(8A)	0.9500	C(20)-C(21)	1.398(8)
C(9)-C(10)	1.400(3)	C(20)-H(20)	0.9500
C(9)-H(9A)	0.9500	C(21)-C(22)	1.373(10)
C(8')-C(9')	1.399(3)	C(21)-H(21)	0.9500
C(8')-H(8B)	0.9500	C(22)-C(23)	1.400(10)
C(9')-C(10)	1.394(3)	C(22)-H(22)	0.9500
C(9')-H(9B)	0.9500	C(23)-C(24)	1.392(8)
C(10)-C(11')	1.388(3)	C(23)-H(23)	0.9500
C(10)-C(11)	1.399(3)	C(24)-H(24)	0.9500
C(10)-H(10)	0.9500	C(25)-C(30)	1.400(8)
C(11)-C(12)	1.377(3)	C(25)-C(26)	1.409(9)
C(11)-H(11A)	0.9500	C(26)-C(27)	1.382(10)
C(12)-H(12A)	0.9500	C(26)-H(26)	0.9500
C(11')-C(12')	1.399(3)	C(27)-C(28)	1.379(11)
C(11')-H(11B)	0.9500	C(27)-H(27)	0.9500
C(12')-H(12B)	0.9500	C(28)-C(29)	1.372(10)
C(13)-C(14)	1.396(3)	C(28)-H(28)	0.9500
C(13)-C(18)	1.396(3)	C(29)-C(30)	1.393(9)
C(14)-C(15)	1.396(3)	C(29)-H(29)	0.9500
C(14)-H(14A)	0.9500	C(30)-H(30)	0.9500
C(15)-C(16)	1.395(3)	C(31)-C(32)	1.393(8)
C(15)-H(15A)	0.9500	C(31)-C(36)	1.412(7)
C(16)-C(17)	1.395(3)	C(32)-C(33)	1.402(8)
C(16)-H(16A)	0.9500	C(32)-H(32)	0.9500
C(17)-C(18)	1.395(3)	C(33)-C(34)	1.383(9)
C(17)-H(17A)	0.9500	C(33)-H(33)	0.9500
C(18)-H(18A)	0.9500	C(34)-C(35)	1.383(9)
C(13')-C(14')	1.396(3)	C(34)-H(34)	0.9500
C(13')-C(18')	1.396(3)	C(35)-C(36)	1.387(8)
C(14')-C(15')	1.396(3)	C(35)-H(35)	0.9500
C(14')-H(14B)	0.9500	C(36)-H(36)	0.9500
C(15')-C(16')	1.394(3)	C(37)-C(42)	1.398(8)
C(15')-H(15B)	0.9500	C(37)-C(38)	1.400(8)
C(16')-C(17')	1.395(3)	C(38)-C(39)	1.388(9)

C(38)-H(38)	0.9500	C(60)-C(61)	1.399(9)
C(39)-C(40)	1.399(10)	C(60)-H(60)	0.9500
C(39)-H(39)	0.9500	C(61)-H(61)	0.9500
C(40)-C(41)	1.380(9)	C(62)-C(63)	1.509(12)
C(40)-H(40)	0.9500	C(62)-H(62A)	0.9900
C(41)-C(42)	1.405(8)	C(62)-H(62B)	0.9900
C(41)-H(41)	0.9500	C(63)-H(63A)	0.9800
C(42)-H(42)	0.9500	C(63)-H(63B)	0.9800
C(43)-C(48)	1.385(8)	C(63)-H(63C)	0.9800
C(43)-C(44)	1.397(8)	C(64)-C(65)	1.521(3)
C(44)-C(45)	1.378(9)	C(64)-H(64A)	0.9900
C(44)-H(44)	0.9500	C(64)-H(64B)	0.9900
C(45)-C(46)	1.375(9)	C(65)-H(65A)	0.9800
C(45)-H(45)	0.9500	C(65)-H(65B)	0.9800
C(46)-C(47)	1.360(9)	C(65)-H(65C)	0.9800
C(46)-H(46)	0.9500	C(64')-C(65')	1.520(3)
C(47)-C(48)	1.391(8)	C(64')-H(64C)	0.9900
C(47)-H(47)	0.9500	C(64')-H(64D)	0.9900
C(48)-H(48)	0.9500	C(65')-H(65D)	0.9800
C(49)-H(49A)	0.9900	C(65')-H(65E)	0.9800
C(49)-H(49B)	0.9900	C(65')-H(65F)	0.9800
C(50)-C(55)	1.395(8)	C(66)-C(71)	1.393(2)
C(50)-C(51)	1.403(9)	C(66)-C(67)	1.395(2)
C(51)-C(52)	1.381(9)	C(66)-C(72)	1.495(2)
C(51)-H(51)	0.9500	C(67)-C(68)	1.395(3)
C(52)-C(53)	1.387(10)	C(67)-H(67)	0.9500
C(52)-H(52)	0.9500	C(68)-C(69)	1.394(3)
C(53)-C(54)	1.389(10)	C(68)-H(68)	0.9500
C(53)-H(53)	0.9500	C(69)-C(70)	1.394(3)
C(54)-C(55)	1.395(9)	C(69)-H(69)	0.9500
C(54)-H(54)	0.9500	C(70)-C(71)	1.397(3)
C(55)-H(55)	0.9500	C(70)-H(70)	0.9500
C(56)-C(57)	1.384(9)	C(71)-H(71)	0.9500
C(56)-C(61)	1.407(8)	C(72)-H(72A)	0.9800
C(57)-C(58)	1.401(10)	C(72)-H(72B)	0.9800
C(57)-H(57)	0.9500	C(72)-H(72C)	0.9800
C(58)-C(59)	1.377(11)	C(73)-C(74)	1.394(2)
C(58)-H(58)	0.9500	C(73)-C(78)	1.395(2)
C(59)-C(60)	1.385(11)	C(73)-C(79)	1.496(2)
C(59)-H(59)	0.9500	C(74)-C(75)	1.396(3)

C(74)-H(74)	0.9500	C(80)-C(86)	1.496(2)
C(75)-C(76)	1.395(3)	C(81)-C(82)	1.396(3)
C(75)-H(75)	0.9500	C(81)-H(81)	0.9500
C(76)-C(77)	1.395(3)	C(82)-C(83)	1.394(3)
C(76)-H(76)	0.9500	C(82)-H(82)	0.9500
C(77)-C(78)	1.396(3)	C(83)-C(84)	1.395(3)
C(77)-H(77)	0.9500	C(83)-H(83)	0.9500
C(78)-H(78)	0.9500	C(84)-C(85)	1.397(3)
C(79)-H(79A)	0.9800	C(84)-H(84)	0.9500
C(79)-H(79B)	0.9800	C(85)-H(85)	0.9500
C(79)-H(79C)	0.9800	C(86)-H(86A)	0.9800
C(80)-C(85)	1.394(2)	C(86)-H(86B)	0.9800
C(80)-C(81)	1.394(3)	C(86)-H(86C)	0.9800
O(7)-Cu(1)-O(10)#1	90.42(15)	O(6)-Si(1)-O(1)	106.57(19)
O(7)-Cu(1)-O(11)#1	171.38(16)	O(7)-Si(1)-C(1)	111.9(2)
O(10)#1-Cu(1)-O(11)#1	95.11(15)	O(6)-Si(1)-C(1)	107.0(2)
O(7)-Cu(1)-O(8)	96.01(15)	O(1)-Si(1)-C(1)	107.8(2)
O(10)#1-Cu(1)-O(8)	172.51(16)	O(8)-Si(2)-O(2)	109.0(2)
O(11)#1-Cu(1)-O(8)	78.96(15)	O(8)-Si(2)-O(1)	109.67(19)
O(12)-Cu(2)-O(8)#1	173.74(16)	O(2)-Si(2)-O(1)	109.25(19)
O(12)-Cu(2)-O(9)#1	88.52(15)	O(8)-Si(2)-C(7)	111.5(2)
O(8)#1-Cu(2)-O(9)#1	96.95(15)	O(2)-Si(2)-C(7)	110.1(2)
O(12)-Cu(2)-O(11)	95.48(15)	O(1)-Si(2)-C(7)	107.3(2)
O(8)#1-Cu(2)-O(11)	79.41(15)	O(9)-Si(3)-O(3)	112.1(2)
O(9)#1-Cu(2)-O(11)	172.78(15)	O(9)-Si(3)-O(2)	112.9(2)
O(13)-P(1)-C(37)	111.9(2)	O(3)-Si(3)-O(2)	107.6(2)
O(13)-P(1)-C(43)	112.1(2)	O(9)-Si(3)-C(13)	111.6(4)
C(37)-P(1)-C(43)	106.9(3)	O(3)-Si(3)-C(13)	105.1(4)
O(13)-P(1)-C(49)	112.1(2)	O(2)-Si(3)-C(13)	107.1(4)
C(37)-P(1)-C(49)	104.3(3)	O(9)-Si(3)-C(13')	112.2(4)
C(43)-P(1)-C(49)	109.2(3)	O(3)-Si(3)-C(13')	106.0(4)
O(14)-P(2)-C(56)	111.7(3)	O(2)-Si(3)-C(13')	105.6(4)
O(14)-P(2)-C(50)	112.0(3)	O(10)-Si(4)-O(3)	112.1(2)
C(56)-P(2)-C(50)	105.7(3)	O(10)-Si(4)-O(4)	111.8(2)
O(14)-P(2)-C(49)	115.6(3)	O(3)-Si(4)-O(4)	109.0(2)
C(56)-P(2)-C(49)	106.2(3)	O(10)-Si(4)-C(19)	110.1(2)
C(50)-P(2)-C(49)	104.9(3)	O(3)-Si(4)-C(19)	106.7(2)
O(7)-Si(1)-O(6)	111.6(2)	O(4)-Si(4)-C(19)	107.0(2)
O(7)-Si(1)-O(1)	111.69(19)	O(11)-Si(5)-O(5)	110.2(2)

O(11)-Si(5)-O(4)	108.8(2)	Si(5)-O(5)-Si(6)	129.9(2)
O(5)-Si(5)-O(4)	110.7(2)	Si(1)-O(6)-Si(6)	137.2(2)
O(11)-Si(5)-C(25)	110.1(2)	Si(1)-O(7)-Cu(1)	134.6(2)
O(5)-Si(5)-C(25)	107.3(2)	Si(1)-O(7)-Na(1)	120.1(2)
O(4)-Si(5)-C(25)	109.8(2)	Cu(1)-O(7)-Na(1)	98.15(16)
O(12)-Si(6)-O(6)	113.6(2)	Si(2)-O(8)-Cu(2)#1	132.8(2)
O(12)-Si(6)-O(5)	110.52(19)	Si(2)-O(8)-Cu(1)	126.7(2)
O(6)-Si(6)-O(5)	107.95(19)	Cu(2)#1-O(8)-Cu(1)	100.07(17)
O(12)-Si(6)-C(31)	112.2(2)	Si(3)-O(9)-Cu(2)#1	129.1(2)
O(6)-Si(6)-C(31)	104.4(2)	Si(3)-O(9)-Na(2)#1	129.8(2)
O(5)-Si(6)-C(31)	107.8(2)	Cu(2)#1-O(9)-Na(2)#1	88.62(15)
O(7)-Na(1)-O(13)	137.51(16)	Si(3)-O(9)-Na(1)#1	123.3(2)
O(7)-Na(1)-O(15)	87.82(16)	Cu(2)#1-O(9)-Na(1)#1	91.22(15)
O(13)-Na(1)-O(15)	95.85(17)	Na(2)#1-O(9)-Na(1)#1	79.86(13)
O(7)-Na(1)-O(9)#1	117.09(15)	Si(4)-O(10)-Cu(1)#1	131.7(2)
O(13)-Na(1)-O(9)#1	91.98(14)	Si(4)-O(10)-Na(1)#1	121.6(2)
O(15)-Na(1)-O(9)#1	130.85(17)	Cu(1)#1-O(10)-Na(1)#1	89.22(14)
O(7)-Na(1)-O(10)#1	67.03(13)	Si(5)-O(11)-Cu(1)#1	128.5(2)
O(13)-Na(1)-O(10)#1	151.50(15)	Si(5)-O(11)-Cu(2)	126.5(2)
O(15)-Na(1)-O(10)#1	66.75(15)	Cu(1)#1-O(11)-Cu(2)	100.04(17)
O(9)#1-Na(1)-O(10)#1	84.18(13)	Si(6)-O(12)-Cu(2)	132.5(2)
O(7)-Na(1)-O(12)	86.00(13)	Si(6)-O(12)-Na(2)	132.2(2)
O(13)-Na(1)-O(12)	79.60(13)	Cu(2)-O(12)-Na(2)	90.94(15)
O(15)-Na(1)-O(12)	164.83(17)	Si(6)-O(12)-Na(1)	114.41(19)
O(9)#1-Na(1)-O(12)	64.10(13)	Cu(2)-O(12)-Na(1)	89.03(15)
O(10)#1-Na(1)-O(12)	122.77(14)	Na(2)-O(12)-Na(1)	79.13(13)
O(14)-Na(2)-O(12)	142.02(18)	P(1)-O(13)-Na(1)	144.9(2)
O(14)-Na(2)-O(13)	87.98(17)	P(1)-O(13)-Na(2)	131.5(2)
O(12)-Na(2)-O(13)	85.04(14)	Na(1)-O(13)-Na(2)	83.54(14)
O(14)-Na(2)-O(9)#1	148.23(18)	P(2)-O(14)-Na(2)	134.8(3)
O(12)-Na(2)-O(9)#1	69.68(14)	C(62)-O(15)-Na(1)	168.2(5)
O(13)-Na(2)-O(9)#1	94.63(15)	C(62)-O(15)-H(15O)	107.8
O(14)-Na(2)-O(16)	94.7(2)	Na(1)-O(15)-H(15O)	73.3
O(12)-Na(2)-O(16)	82.5(2)	C(64')-O(16)-Na(2)	128.2(16)
O(13)-Na(2)-O(16)	162.9(2)	C(64)-O(16)-Na(2)	119.1(6)
O(9)#1-Na(2)-O(16)	91.9(2)	C(64')-O(16)-H(16O)	114.1
Si(2)-O(1)-Si(1)	126.0(2)	C(64)-O(16)-H(16O)	114.2
Si(2)-O(2)-Si(3)	132.2(2)	Na(2)-O(16)-H(16O)	114.2
Si(3)-O(3)-Si(4)	143.8(2)	C(2)-C(1)-C(6)	117.0(5)
Si(5)-O(4)-Si(4)	129.6(2)	C(2)-C(1)-Si(1)	121.4(4)

C(6)-C(1)-Si(1)	121.6(4)	C(10)-C(11)-H(11A)	118.6
C(1)-C(2)-C(3)	121.7(6)	C(7)-C(12)-C(11)	117.7(2)
C(1)-C(2)-H(2)	119.1	C(7)-C(12)-H(12A)	121.1
C(3)-C(2)-H(2)	119.1	C(11)-C(12)-H(12A)	121.1
C(4)-C(3)-C(2)	120.1(6)	C(10)-C(11')-C(12')	119.5(2)
C(4)-C(3)-H(3)	119.9	C(10)-C(11')-H(11B)	120.2
C(2)-C(3)-H(3)	119.9	C(12')-C(11')-H(11B)	120.2
C(3)-C(4)-C(5)	119.6(6)	C(7)-C(12')-C(11')	119.6(2)
C(3)-C(4)-H(4)	120.2	C(7)-C(12')-H(12B)	120.2
C(5)-C(4)-H(4)	120.2	C(11')-C(12')-H(12B)	120.2
C(6)-C(5)-C(4)	119.5(6)	C(14)-C(13)-C(18)	119.9(2)
C(6)-C(5)-H(5)	120.3	C(14)-C(13)-Si(3)	123.3(7)
C(4)-C(5)-H(5)	120.3	C(18)-C(13)-Si(3)	116.5(7)
C(5)-C(6)-C(1)	122.1(6)	C(13)-C(14)-C(15)	120.0(2)
C(5)-C(6)-H(6)	119.0	C(13)-C(14)-H(14A)	120.0
C(1)-C(6)-H(6)	119.0	C(15)-C(14)-H(14A)	120.0
C(12')-C(7)-C(8')	120.86(19)	C(16)-C(15)-C(14)	119.9(2)
C(12)-C(7)-C(8)	122.1(2)	C(16)-C(15)-H(15A)	120.0
C(12)-C(7)-Si(2)	119.7(3)	C(14)-C(15)-H(15A)	120.0
C(12')-C(7)-Si(2)	117.8(3)	C(15)-C(16)-C(17)	120.1(2)
C(8')-C(7)-Si(2)	121.2(3)	C(15)-C(16)-H(16A)	120.0
C(8)-C(7)-Si(2)	118.1(3)	C(17)-C(16)-H(16A)	120.0
C(7)-C(8)-C(9)	119.8(2)	C(18)-C(17)-C(16)	119.9(2)
C(7)-C(8)-H(8A)	120.1	C(18)-C(17)-H(17A)	120.0
C(9)-C(8)-H(8A)	120.1	C(16)-C(17)-H(17A)	120.0
C(8)-C(9)-C(10)	118.9(2)	C(17)-C(18)-C(13)	120.0(2)
C(8)-C(9)-H(9A)	120.5	C(17)-C(18)-H(18A)	120.0
C(10)-C(9)-H(9A)	120.5	C(13)-C(18)-H(18A)	120.0
C(7)-C(8')-C(9')	119.5(2)	C(14')-C(13')-C(18')	119.9(2)
C(7)-C(8')-H(8B)	120.2	C(14')-C(13')-Si(3)	118.8(6)
C(9')-C(8')-H(8B)	120.2	C(18')-C(13')-Si(3)	121.3(6)
C(10)-C(9')-C(8')	119.4(2)	C(13')-C(14')-C(15')	120.0(2)
C(10)-C(9')-H(9B)	120.3	C(13')-C(14')-H(14B)	120.0
C(8')-C(9')-H(9B)	120.3	C(15')-C(14')-H(14B)	120.0
C(11')-C(10)-C(9')	121.07(19)	C(16')-C(15')-C(14')	120.0(2)
C(11)-C(10)-C(9)	118.56(18)	C(16')-C(15')-H(15B)	120.0
C(11)-C(10)-H(10)	120.7	C(14')-C(15')-H(15B)	120.0
C(9)-C(10)-H(10)	120.7	C(15')-C(16')-C(17')	120.0(2)
C(12)-C(11)-C(10)	122.9(2)	C(15')-C(16')-H(16B)	120.0
C(12)-C(11)-H(11A)	118.6	C(17')-C(16')-H(16B)	120.0

C(16')-C(17')-C(18')	120.0(2)	C(29)-C(30)-H(30)	119.4
C(16')-C(17')-H(17B)	120.0	C(25)-C(30)-H(30)	119.4
C(18')-C(17')-H(17B)	120.0	C(32)-C(31)-C(36)	117.5(5)
C(17')-C(18')-C(13')	120.1(2)	C(32)-C(31)-Si(6)	122.3(4)
C(17')-C(18')-H(18B)	120.0	C(36)-C(31)-Si(6)	120.1(4)
C(13')-C(18')-H(18B)	120.0	C(31)-C(32)-C(33)	121.0(6)
C(24)-C(19)-C(20)	117.2(5)	C(31)-C(32)-H(32)	119.5
C(24)-C(19)-Si(4)	121.8(4)	C(33)-C(32)-H(32)	119.5
C(20)-C(19)-Si(4)	120.9(4)	C(34)-C(33)-C(32)	120.3(6)
C(21)-C(20)-C(19)	121.5(6)	C(34)-C(33)-H(33)	119.9
C(21)-C(20)-H(20)	119.2	C(32)-C(33)-H(33)	119.9
C(19)-C(20)-H(20)	119.2	C(33)-C(34)-C(35)	119.7(5)
C(22)-C(21)-C(20)	120.1(6)	C(33)-C(34)-H(34)	120.2
C(22)-C(21)-H(21)	120.0	C(35)-C(34)-H(34)	120.2
C(20)-C(21)-H(21)	120.0	C(34)-C(35)-C(36)	120.3(6)
C(21)-C(22)-C(23)	119.9(6)	C(34)-C(35)-H(35)	119.8
C(21)-C(22)-H(22)	120.1	C(36)-C(35)-H(35)	119.8
C(23)-C(22)-H(22)	120.1	C(35)-C(36)-C(31)	121.2(6)
C(24)-C(23)-C(22)	119.9(6)	C(35)-C(36)-H(36)	119.4
C(24)-C(23)-H(23)	120.1	C(31)-C(36)-H(36)	119.4
C(22)-C(23)-H(23)	120.1	C(42)-C(37)-C(38)	119.0(6)
C(23)-C(24)-C(19)	121.4(6)	C(42)-C(37)-P(1)	118.3(4)
C(23)-C(24)-H(24)	119.3	C(38)-C(37)-P(1)	122.7(4)
C(19)-C(24)-H(24)	119.3	C(39)-C(38)-C(37)	120.6(6)
C(30)-C(25)-C(26)	117.2(6)	C(39)-C(38)-H(38)	119.7
C(30)-C(25)-Si(5)	121.5(5)	C(37)-C(38)-H(38)	119.7
C(26)-C(25)-Si(5)	121.3(5)	C(38)-C(39)-C(40)	119.8(6)
C(27)-C(26)-C(25)	120.8(7)	C(38)-C(39)-H(39)	120.1
C(27)-C(26)-H(26)	119.6	C(40)-C(39)-H(39)	120.1
C(25)-C(26)-H(26)	119.6	C(41)-C(40)-C(39)	120.4(6)
C(28)-C(27)-C(26)	120.8(7)	C(41)-C(40)-H(40)	119.8
C(28)-C(27)-H(27)	119.6	C(39)-C(40)-H(40)	119.8
C(26)-C(27)-H(27)	119.6	C(40)-C(41)-C(42)	119.8(6)
C(29)-C(28)-C(27)	119.6(7)	C(40)-C(41)-H(41)	120.1
C(29)-C(28)-H(28)	120.2	C(42)-C(41)-H(41)	120.1
C(27)-C(28)-H(28)	120.2	C(37)-C(42)-C(41)	120.4(6)
C(28)-C(29)-C(30)	120.4(7)	C(37)-C(42)-H(42)	119.8
C(28)-C(29)-H(29)	119.8	C(41)-C(42)-H(42)	119.8
C(30)-C(29)-H(29)	119.8	C(48)-C(43)-C(44)	118.3(5)
C(29)-C(30)-C(25)	121.1(6)	C(48)-C(43)-P(1)	124.5(4)

C(44)-C(43)-P(1)	117.1(4)	C(57)-C(56)-C(61)	119.6(6)
C(45)-C(44)-C(43)	119.7(6)	C(57)-C(56)-P(2)	118.4(5)
C(45)-C(44)-H(44)	120.1	C(61)-C(56)-P(2)	122.0(5)
C(43)-C(44)-H(44)	120.1	C(56)-C(57)-C(58)	119.9(7)
C(46)-C(45)-C(44)	121.2(7)	C(56)-C(57)-H(57)	120.0
C(46)-C(45)-H(45)	119.4	C(58)-C(57)-H(57)	120.0
C(44)-C(45)-H(45)	119.4	C(59)-C(58)-C(57)	120.0(8)
C(47)-C(46)-C(45)	119.6(6)	C(59)-C(58)-H(58)	120.0
C(47)-C(46)-H(46)	120.2	C(57)-C(58)-H(58)	120.0
C(45)-C(46)-H(46)	120.2	C(58)-C(59)-C(60)	121.1(7)
C(46)-C(47)-C(48)	120.2(6)	C(58)-C(59)-H(59)	119.4
C(46)-C(47)-H(47)	119.9	C(60)-C(59)-H(59)	119.4
C(48)-C(47)-H(47)	119.9	C(59)-C(60)-C(61)	119.1(7)
C(43)-C(48)-C(47)	120.8(6)	C(59)-C(60)-H(60)	120.4
C(43)-C(48)-H(48)	119.6	C(61)-C(60)-H(60)	120.4
C(47)-C(48)-H(48)	119.6	C(60)-C(61)-C(56)	120.2(7)
P(1)-C(49)-P(2)	116.6(3)	C(60)-C(61)-H(61)	119.9
P(1)-C(49)-H(49A)	108.2	C(56)-C(61)-H(61)	119.9
P(2)-C(49)-H(49A)	108.2	O(15)-C(62)-C(63)	112.0(9)
P(1)-C(49)-H(49B)	108.2	O(15)-C(62)-H(62A)	109.2
P(2)-C(49)-H(49B)	108.2	C(63)-C(62)-H(62A)	109.2
H(49A)-C(49)-H(49B)	107.3	O(15)-C(62)-H(62B)	109.2
C(55)-C(50)-C(51)	118.5(6)	C(63)-C(62)-H(62B)	109.2
C(55)-C(50)-P(2)	117.5(5)	H(62A)-C(62)-H(62B)	107.9
C(51)-C(50)-P(2)	124.0(5)	C(62)-C(63)-H(63A)	109.5
C(52)-C(51)-C(50)	120.5(6)	C(62)-C(63)-H(63B)	109.5
C(52)-C(51)-H(51)	119.7	H(63A)-C(63)-H(63B)	109.5
C(50)-C(51)-H(51)	119.7	C(62)-C(63)-H(63C)	109.5
C(51)-C(52)-C(53)	120.0(7)	H(63A)-C(63)-H(63C)	109.5
C(51)-C(52)-H(52)	120.0	H(63B)-C(63)-H(63C)	109.5
C(53)-C(52)-H(52)	120.0	O(16)-C(64)-C(65)	111.8(3)
C(52)-C(53)-C(54)	120.8(7)	O(16)-C(64)-H(64A)	109.3
C(52)-C(53)-H(53)	119.6	C(65)-C(64)-H(64A)	109.3
C(54)-C(53)-H(53)	119.6	O(16)-C(64)-H(64B)	109.3
C(53)-C(54)-C(55)	118.7(7)	C(65)-C(64)-H(64B)	109.3
C(53)-C(54)-H(54)	120.6	H(64A)-C(64)-H(64B)	107.9
C(55)-C(54)-H(54)	120.6	C(64)-C(65)-H(65A)	109.5
C(50)-C(55)-C(54)	121.3(6)	C(64)-C(65)-H(65B)	109.5
C(50)-C(55)-H(55)	119.4	H(65A)-C(65)-H(65B)	109.5
C(54)-C(55)-H(55)	119.4	C(64)-C(65)-H(65C)	109.5

H(65A)-C(65)-H(65C)	109.5	C(78)-C(73)-C(79)	119.7(2)
H(65B)-C(65)-H(65C)	109.5	C(73)-C(74)-C(75)	119.9(2)
O(16)-C(64')-C(65')	112.3(3)	C(73)-C(74)-H(74)	120.1
O(16)-C(64')-H(64C)	109.1	C(75)-C(74)-H(74)	120.1
C(65')-C(64')-H(64C)	109.1	C(76)-C(75)-C(74)	120.0(2)
O(16)-C(64')-H(64D)	109.1	C(76)-C(75)-H(75)	120.0
C(65')-C(64')-H(64D)	109.1	C(74)-C(75)-H(75)	120.0
H(64C)-C(64')-H(64D)	107.9	C(75)-C(76)-C(77)	120.1(2)
C(64')-C(65')-H(65D)	109.5	C(75)-C(76)-H(76)	119.9
C(64')-C(65')-H(65E)	109.5	C(77)-C(76)-H(76)	119.9
H(65D)-C(65')-H(65E)	109.5	C(76)-C(77)-C(78)	119.9(2)
C(64')-C(65')-H(65F)	109.5	C(76)-C(77)-H(77)	120.0
H(65D)-C(65')-H(65F)	109.5	C(78)-C(77)-H(77)	120.0
H(65E)-C(65')-H(65F)	109.5	C(73)-C(78)-C(77)	119.9(2)
C(71)-C(66)-C(67)	120.2(2)	C(73)-C(78)-H(78)	120.0
C(71)-C(66)-C(72)	119.9(2)	C(77)-C(78)-H(78)	120.0
C(67)-C(66)-C(72)	119.9(2)	C(73)-C(79)-H(79A)	109.5
C(66)-C(67)-C(68)	119.9(2)	C(73)-C(79)-H(79B)	109.5
C(66)-C(67)-H(67)	120.1	H(79A)-C(79)-H(79B)	109.5
C(68)-C(67)-H(67)	120.1	C(73)-C(79)-H(79C)	109.5
C(69)-C(68)-C(67)	120.0(2)	H(79A)-C(79)-H(79C)	109.5
C(69)-C(68)-H(68)	120.0	H(79B)-C(79)-H(79C)	109.5
C(67)-C(68)-H(68)	120.0	C(85)-C(80)-C(81)	120.2(2)
C(70)-C(69)-C(68)	120.1(2)	C(85)-C(80)-C(86)	119.9(2)
C(70)-C(69)-H(69)	120.0	C(81)-C(80)-C(86)	119.8(2)
C(68)-C(69)-H(69)	120.0	C(80)-C(81)-C(82)	119.9(2)
C(69)-C(70)-C(71)	119.9(2)	C(80)-C(81)-H(81)	120.1
C(69)-C(70)-H(70)	120.0	C(82)-C(81)-H(81)	120.1
C(71)-C(70)-H(70)	120.0	C(83)-C(82)-C(81)	120.0(2)
C(66)-C(71)-C(70)	119.9(2)	C(83)-C(82)-H(82)	120.0
C(66)-C(71)-H(71)	120.0	C(81)-C(82)-H(82)	120.0
C(70)-C(71)-H(71)	120.0	C(82)-C(83)-C(84)	120.2(2)
C(66)-C(72)-H(72A)	109.5	C(82)-C(83)-H(83)	119.9
C(66)-C(72)-H(72B)	109.5	C(84)-C(83)-H(83)	119.9
H(72A)-C(72)-H(72B)	109.5	C(83)-C(84)-C(85)	119.9(2)
C(66)-C(72)-H(72C)	109.5	C(83)-C(84)-H(84)	120.1
H(72A)-C(72)-H(72C)	109.5	C(85)-C(84)-H(84)	120.0
H(72B)-C(72)-H(72C)	109.5	C(80)-C(85)-C(84)	119.9(2)
C(74)-C(73)-C(78)	120.2(2)	C(80)-C(85)-H(85)	120.1
C(74)-C(73)-C(79)	120.1(2)	C(84)-C(85)-H(85)	120.1

C(80)-C(86)-H(86A)	109.5	C(80)-C(86)-H(86C)	109.5
C(80)-C(86)-H(86B)	109.5	H(86A)-C(86)-H(86C)	109.5
H(86A)-C(86)-H(86B)	109.5	H(86B)-C(86)-H(86C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1, -y+1, -z+1$

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	36(1)	25(1)	27(1)	-1(1)	2(1)	1(1)
Cu(2)	34(1)	26(1)	28(1)	0(1)	3(1)	1(1)
P(1)	37(1)	29(1)	36(1)	3(1)	3(1)	3(1)
P(2)	43(1)	39(1)	38(1)	4(1)	10(1)	1(1)
Si(1)	34(1)	28(1)	27(1)	-1(1)	3(1)	0(1)
Si(2)	36(1)	29(1)	26(1)	-1(1)	4(1)	3(1)
Si(3)	41(1)	28(1)	31(1)	-1(1)	5(1)	4(1)
Si(4)	45(1)	27(1)	28(1)	-1(1)	5(1)	-2(1)
Si(5)	44(1)	30(1)	27(1)	-2(1)	3(1)	-2(1)
Si(6)	35(1)	29(1)	26(1)	0(1)	3(1)	0(1)
Na(1)	38(1)	31(1)	36(1)	1(1)	4(1)	6(1)
Na(2)	36(1)	38(1)	36(1)	4(1)	6(1)	6(1)
O(1)	38(2)	26(2)	33(2)	-4(2)	5(2)	-2(2)
O(2)	43(2)	29(2)	34(2)	-4(2)	6(2)	3(2)
O(3)	51(2)	34(2)	34(2)	-7(2)	7(2)	-1(2)
O(4)	51(2)	27(2)	29(2)	-4(2)	2(2)	-3(2)
O(5)	37(2)	33(2)	30(2)	-4(2)	1(2)	-3(2)
O(6)	43(2)	33(2)	25(2)	0(2)	4(2)	1(2)
O(7)	37(2)	26(2)	41(2)	2(2)	7(2)	6(2)
O(8)	40(2)	34(2)	36(2)	1(2)	4(2)	2(2)
O(9)	39(2)	35(2)	31(2)	3(2)	2(2)	3(2)
O(10)	46(2)	35(2)	31(2)	1(2)	5(2)	0(2)
O(11)	45(2)	35(2)	35(2)	1(2)	2(2)	2(2)
O(12)	36(2)	30(2)	39(2)	3(2)	8(2)	4(2)
O(13)	35(2)	34(2)	40(2)	3(2)	3(2)	3(2)
O(14)	57(3)	64(3)	58(3)	8(2)	10(2)	8(2)
O(15)	74(3)	49(3)	59(3)	3(2)	12(2)	-16(2)
O(16)	125(5)	125(5)	114(5)	-19(4)	65(4)	-42(4)
C(1)	33(3)	32(3)	38(3)	-1(2)	2(2)	4(2)
C(2)	52(4)	41(3)	42(3)	-3(3)	5(3)	-7(3)
C(3)	53(4)	52(4)	60(4)	7(3)	12(3)	-16(3)
C(4)	43(3)	57(4)	51(4)	12(3)	18(3)	-3(3)
C(5)	53(4)	53(4)	40(3)	-1(3)	17(3)	2(3)
C(6)	50(3)	40(3)	43(3)	-3(3)	13(3)	-7(3)
C(7)	42(3)	37(3)	35(3)	0(2)	6(2)	8(2)

C(8)	48(7)	45(7)	61(9)	0(6)	12(6)	-4(6)
C(9)	51(9)	53(9)	148(18)	7(10)	34(10)	-3(7)
C(8')	68(10)	116(15)	46(8)	-15(9)	16(7)	-28(10)
C(9')	52(10)	130(18)	109(16)	-25(14)	17(10)	-37(11)
C(10)	60(5)	99(7)	106(7)	36(6)	40(5)	-7(5)
C(11)	38(8)	129(16)	72(11)	0(11)	26(7)	9(9)
C(12)	51(7)	43(7)	52(8)	-13(6)	5(6)	-1(6)
C(11')	61(10)	137(17)	49(9)	23(10)	16(8)	13(10)
C(12')	52(8)	94(12)	50(8)	1(8)	14(7)	12(8)
C(13)	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(14)	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(15)	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(16)	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(17)	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(18)	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(13')	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(14')	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(15')	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(16')	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(17')	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(18')	73(3)	41(2)	59(2)	2(2)	17(2)	14(2)
C(19)	51(3)	32(3)	28(3)	-4(2)	7(2)	0(2)
C(20)	58(4)	32(3)	46(3)	3(3)	2(3)	-4(3)
C(21)	79(5)	34(3)	51(4)	6(3)	2(3)	-8(3)
C(22)	83(5)	38(3)	45(4)	-4(3)	15(3)	-19(3)
C(23)	60(4)	53(4)	55(4)	-6(3)	11(3)	-20(3)
C(24)	52(4)	33(3)	49(4)	-1(3)	5(3)	-7(3)
C(25)	55(4)	34(3)	39(3)	-6(2)	8(3)	-4(3)
C(26)	63(4)	60(4)	52(4)	0(3)	19(3)	-10(3)
C(27)	74(5)	87(6)	67(5)	4(4)	34(4)	-11(4)
C(28)	53(4)	86(6)	76(5)	-11(5)	24(4)	-16(4)
C(29)	47(4)	76(5)	65(5)	-12(4)	7(3)	-8(3)
C(30)	47(3)	51(4)	46(4)	-5(3)	9(3)	-9(3)
C(31)	40(3)	26(3)	37(3)	-2(2)	9(2)	-2(2)
C(32)	42(3)	30(3)	41(3)	2(2)	6(2)	1(2)
C(33)	37(3)	42(3)	53(4)	1(3)	-5(3)	4(2)
C(34)	50(4)	40(3)	45(4)	7(3)	-10(3)	1(3)
C(35)	51(4)	54(4)	35(3)	9(3)	-2(3)	-2(3)
C(36)	39(3)	40(3)	32(3)	6(2)	3(2)	1(2)
C(37)	37(3)	32(3)	40(3)	4(2)	1(2)	1(2)

C(38)	60(4)	40(3)	56(4)	5(3)	16(3)	5(3)
C(39)	68(5)	51(4)	67(5)	15(3)	28(4)	4(3)
C(40)	51(4)	71(5)	59(4)	9(4)	24(3)	7(3)
C(41)	50(4)	54(4)	56(4)	6(3)	15(3)	14(3)
C(42)	46(3)	37(3)	42(3)	4(3)	7(3)	3(3)
C(43)	40(3)	36(3)	36(3)	2(2)	3(2)	4(2)
C(44)	73(5)	35(3)	68(5)	-1(3)	-23(4)	8(3)
C(45)	104(6)	42(4)	67(5)	-6(4)	-34(4)	6(4)
C(46)	81(5)	36(3)	54(4)	-7(3)	-8(4)	6(3)
C(47)	62(4)	32(3)	46(4)	3(3)	3(3)	6(3)
C(48)	53(4)	37(3)	37(3)	6(2)	4(3)	0(3)
C(49)	50(3)	29(3)	33(3)	2(2)	3(2)	3(2)
C(50)	42(3)	49(3)	40(3)	8(3)	10(3)	2(3)
C(51)	52(4)	71(5)	49(4)	7(3)	5(3)	-16(3)
C(52)	57(5)	115(7)	49(4)	3(4)	-2(3)	-26(5)
C(53)	49(4)	95(6)	69(5)	-5(5)	2(4)	-22(4)
C(54)	45(4)	75(5)	67(5)	6(4)	13(3)	-10(3)
C(55)	45(4)	63(4)	50(4)	9(3)	10(3)	-1(3)
C(56)	46(3)	47(3)	43(3)	11(3)	13(3)	6(3)
C(57)	90(6)	51(4)	45(4)	7(3)	15(4)	28(4)
C(58)	127(8)	60(5)	63(5)	-4(4)	20(5)	40(5)
C(59)	102(7)	48(4)	90(6)	8(4)	28(5)	29(4)
C(60)	63(4)	51(4)	75(5)	18(4)	16(4)	21(3)
C(61)	46(3)	53(4)	50(4)	16(3)	10(3)	8(3)
C(62)	141(9)	67(5)	80(6)	0(5)	52(6)	-16(6)
C(63)	119(8)	92(7)	82(7)	14(6)	24(6)	-4(6)
C(64)	125(5)	125(5)	114(5)	-19(4)	65(4)	-42(4)
C(65)	125(5)	125(5)	114(5)	-19(4)	65(4)	-42(4)
C(64')	125(5)	125(5)	114(5)	-19(4)	65(4)	-42(4)
C(65')	125(5)	125(5)	114(5)	-19(4)	65(4)	-42(4)
C(66)	122(4)	139(4)	117(4)	-26(3)	21(3)	26(3)
C(67)	122(4)	139(4)	117(4)	-26(3)	21(3)	26(3)
C(68)	122(4)	139(4)	117(4)	-26(3)	21(3)	26(3)
C(69)	122(4)	139(4)	117(4)	-26(3)	21(3)	26(3)
C(70)	122(4)	139(4)	117(4)	-26(3)	21(3)	26(3)
C(71)	122(4)	139(4)	117(4)	-26(3)	21(3)	26(3)
C(72)	122(4)	139(4)	117(4)	-26(3)	21(3)	26(3)
C(73)	74(5)	110(6)	163(9)	-17(6)	28(5)	-15(5)
C(74)	74(5)	110(6)	163(9)	-17(6)	28(5)	-15(5)
C(75)	74(5)	110(6)	163(9)	-17(6)	28(5)	-15(5)

C(76)	74(5)	110(6)	163(9)	-17(6)	28(5)	-15(5)
C(77)	74(5)	110(6)	163(9)	-17(6)	28(5)	-15(5)
C(78)	74(5)	110(6)	163(9)	-17(6)	28(5)	-15(5)
C(79)	74(5)	110(6)	163(9)	-17(6)	28(5)	-15(5)
C(80)	76(7)	100(9)	68(5)	-5(5)	5(4)	-10(5)
C(81)	76(7)	100(9)	68(5)	-5(5)	5(4)	-10(5)
C(82)	76(7)	100(9)	68(5)	-5(5)	5(4)	-10(5)
C(83)	76(7)	100(9)	68(5)	-5(5)	5(4)	-10(5)
C(84)	76(7)	100(9)	68(5)	-5(5)	5(4)	-10(5)
C(85)	76(7)	100(9)	68(5)	-5(5)	5(4)	-10(5)
C(86)	76(7)	100(9)	68(5)	-5(5)	5(4)	-10(5)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.

Atom	x	y	z	U(iso)
H(15O)	4311	3145	5931	91
H(16O)	8282	4762	5993	175
H(2)	3623	3769	7026	55
H(3)	2902	3455	7794	66
H(4)	2991	3931	8739	59
H(5)	3785	4742	8901	57
H(6)	4479	5062	8120	53
H(8A)	2655	4499	6008	61
H(9A)	1413	4202	6308	99
H(8B)	2018	5063	5408	91
H(9B)	776	4768	5709	116
H(10)	606	4851	6759	102
H(11A)	1066	5767	6895	93
H(12A)	2289	6059	6598	59
H(11B)	1659	5199	7506	98
H(12B)	2900	5493	7205	78
H(14A)	2695	7086	6139	68
H(15A)	1969	7926	6079	68
H(16A)	1950	8506	5210	68
H(17A)	2659	8249	4402	68
H(18A)	3386	7409	4463	68
H(14B)	2517	6924	6049	68
H(15B)	1592	7667	6011	68
H(16B)	1591	8367	5261	68
H(17B)	2518	8324	4550	68
H(18B)	3443	7581	4588	68
H(20)	5074	7791	4891	55
H(21)	5655	8653	4736	67
H(22)	7049	8808	5080	66
H(23)	7873	8102	5606	66
H(24)	7304	7234	5741	54
H(26)	7643	6143	5076	69
H(27)	9029	6219	5002	88
H(28)	10040	6018	5855	84
H(29)	9663	5762	6799	75
H(30)	8276	5678	6889	57

H(32)	8308	4606	7147	45
H(33)	9288	4421	8036	55
H(34)	8893	4363	9018	57
H(35)	7519	4508	9117	57
H(36)	6543	4710	8242	45
H(38)	6348	2076	8239	61
H(39)	5507	2186	8998	72
H(40)	4918	3053	9139	70
H(41)	5134	3798	8505	63
H(42)	5966	3687	7730	50
H(44)	5809	2279	6351	75
H(45)	5666	1390	5937	92
H(46)	6541	682	6353	71
H(47)	7543	851	7212	57
H(48)	7680	1734	7657	51
H(49A)	8061	2629	8041	45
H(49B)	7932	3282	7960	45
H(51)	9418	2965	8602	69
H(52)	10595	3344	9196	90
H(53)	11488	3884	8719	87
H(54)	11243	4021	7636	74
H(55)	10077	3617	7035	63
H(57)	8660	2269	6185	74
H(58)	8928	1331	6005	100
H(59)	9456	758	6833	94
H(60)	9771	1107	7847	75
H(61)	9493	2043	8036	59
H(62A)	3728	2328	6134	111
H(62B)	3371	2858	6444	111
H(63A)	3661	2115	7166	145
H(63B)	4175	2658	7406	145
H(63C)	4615	2159	7105	145
H(64A)	9446	4285	5895	140
H(64B)	9106	4585	5246	140
H(65A)	9083	3771	4808	175
H(65B)	8325	3618	5151	175
H(65C)	9245	3465	5471	175
H(64C)	8050	4792	4928	140
H(64D)	8304	4152	4924	140
H(65D)	9389	4739	4715	175

H(65E)	9675	4374	5328	175
H(65F)	9435	5011	5392	175
H(67)	2346	5396	8840	151
H(68)	2802	4789	9670	151
H(69)	1847	4371	10214	151
H(70)	437	4560	9931	151
H(71)	-18	5167	9099	151
H(72A)	411	5974	8480	189
H(72B)	593	5510	7993	189
H(72C)	1297	5943	8269	189
H(74)	3635	7606	7546	138
H(75)	3480	6684	7201	138
H(76)	3175	5989	7883	138
H(77)	3022	6214	8908	138
H(78)	3178	7135	9254	138
H(79A)	3272	8087	9033	172
H(79B)	3242	8292	8328	172
H(79C)	4106	8137	8748	172
H(81)	5081	5772	9448	99
H(82)	6014	5088	9241	99
H(83)	6033	4222	9732	99
H(84)	5121	4037	10430	99
H(85)	4188	4722	10637	99
H(86A)	4140	6110	10073	123
H(86B)	3922	5748	10641	123
H(86C)	3407	5668	9954	123

Table S6. Torsion angles [°] for **1**.

O(8)-Si(2)-O(1)-Si(1)	-45.0(3)	O(5)-Si(6)-O(6)-Si(1)	83.4(4)
O(2)-Si(2)-O(1)-Si(1)	-164.5(3)	C(31)-Si(6)-O(6)-Si(1)	-162.1(3)
C(7)-Si(2)-O(1)-Si(1)	76.2(3)	O(6)-Si(1)-O(7)-Cu(1)	-118.3(3)
O(7)-Si(1)-O(1)-Si(2)	24.4(3)	O(1)-Si(1)-O(7)-Cu(1)	0.9(4)
O(6)-Si(1)-O(1)-Si(2)	146.6(3)	C(1)-Si(1)-O(7)-Cu(1)	121.8(3)
C(1)-Si(1)-O(1)-Si(2)	-98.9(3)	Na(1)-Si(1)-O(7)-Cu(1)	-143.2(4)
Na(1)-Si(1)-O(1)-Si(2)	55.5(4)	O(6)-Si(1)-O(7)-Na(1)	24.9(3)
O(8)-Si(2)-O(2)-Si(3)	-0.3(4)	O(1)-Si(1)-O(7)-Na(1)	144.0(2)
O(1)-Si(2)-O(2)-Si(3)	119.5(3)	C(1)-Si(1)-O(7)-Na(1)	-95.0(3)
C(7)-Si(2)-O(2)-Si(3)	-122.9(3)	O(10)#1-Cu(1)-O(7)-Si(1)	-177.8(3)
O(9)-Si(3)-O(2)-Si(2)	20.8(4)	O(8)-Cu(1)-O(7)-Si(1)	-1.7(3)
O(3)-Si(3)-O(2)-Si(2)	-103.4(3)	Cu(2)#1-Cu(1)-O(7)-Si(1)	12.8(4)
C(13)-Si(3)-O(2)-Si(2)	144.0(5)	Na(1)-Cu(1)-O(7)-Si(1)	148.4(4)
C(13')-Si(3)-O(2)-Si(2)	143.7(5)	O(10)#1-Cu(1)-O(7)-Na(1)	33.80(16)
O(9)-Si(3)-O(3)-Si(4)	-23.9(5)	O(8)-Cu(1)-O(7)-Na(1)	-150.05(15)
O(2)-Si(3)-O(3)-Si(4)	100.8(4)	Cu(2)#1-Cu(1)-O(7)-Na(1)	-135.65(10)
C(13)-Si(3)-O(3)-Si(4)	-145.3(6)	O(2)-Si(2)-O(8)-Cu(2)#1	-25.0(4)
C(13')-Si(3)-O(3)-Si(4)	-146.6(6)	O(1)-Si(2)-O(8)-Cu(2)#1	-144.6(3)
O(10)-Si(4)-O(3)-Si(3)	22.7(5)	C(7)-Si(2)-O(8)-Cu(2)#1	96.7(3)
O(4)-Si(4)-O(3)-Si(3)	-101.5(4)	O(2)-Si(2)-O(8)-Cu(1)	163.6(2)
C(19)-Si(4)-O(3)-Si(3)	143.3(4)	O(1)-Si(2)-O(8)-Cu(1)	44.1(3)
O(11)-Si(5)-O(4)-Si(4)	-24.2(4)	C(7)-Si(2)-O(8)-Cu(1)	-74.6(3)
O(5)-Si(5)-O(4)-Si(4)	-145.4(3)	O(3)-Si(3)-O(9)-Cu(2)#1	100.8(3)
C(25)-Si(5)-O(4)-Si(4)	96.4(3)	O(2)-Si(3)-O(9)-Cu(2)#1	-20.9(4)
O(10)-Si(4)-O(4)-Si(5)	-6.2(4)	C(13)-Si(3)-O(9)-Cu(2)#1	-141.6(5)
O(3)-Si(4)-O(4)-Si(5)	118.3(3)	C(13')-Si(3)-O(9)-Cu(2)#1	-140.0(5)
C(19)-Si(4)-O(4)-Si(5)	-126.8(3)	O(3)-Si(3)-O(9)-Na(2)#1	-129.6(3)
O(11)-Si(5)-O(5)-Si(6)	22.1(4)	O(2)-Si(3)-O(9)-Na(2)#1	108.8(3)
O(4)-Si(5)-O(5)-Si(6)	142.5(3)	C(13)-Si(3)-O(9)-Na(2)#1	-12.0(5)
C(25)-Si(5)-O(5)-Si(6)	-97.8(3)	C(13')-Si(3)-O(9)-Na(2)#1	-10.4(5)
O(12)-Si(6)-O(5)-Si(5)	9.4(4)	O(3)-Si(3)-O(9)-Na(1)#1	-23.7(3)
O(6)-Si(6)-O(5)-Si(5)	-115.3(3)	O(2)-Si(3)-O(9)-Na(1)#1	-145.4(2)
C(31)-Si(6)-O(5)-Si(5)	132.4(3)	C(13)-Si(3)-O(9)-Na(1)#1	93.9(5)
O(7)-Si(1)-O(6)-Si(6)	38.9(4)	C(13')-Si(3)-O(9)-Na(1)#1	95.4(5)
O(1)-Si(1)-O(6)-Si(6)	-83.3(4)	O(3)-Si(4)-O(10)-Cu(1)#1	-97.6(3)
C(1)-Si(1)-O(6)-Si(6)	161.6(3)	O(4)-Si(4)-O(10)-Cu(1)#1	25.0(4)
Na(1)-Si(1)-O(6)-Si(6)	53.5(3)	C(19)-Si(4)-O(10)-Cu(1)#1	143.8(3)
O(12)-Si(6)-O(6)-Si(1)	-39.5(4)	O(3)-Si(4)-O(10)-Na(1)#1	24.2(3)

O(4)-Si(4)-O(10)-Na(1)#1	146.8(2)	C(2)-C(1)-C(6)-C(5)	-0.4(9)
C(19)-Si(4)-O(10)-Na(1)#1	-94.4(3)	Si(1)-C(1)-C(6)-C(5)	178.4(5)
O(5)-Si(5)-O(11)-Cu(1)#1	166.1(2)	O(9)-Si(3)-C(13)-C(18)	-50.3(6)
O(4)-Si(5)-O(11)-Cu(1)#1	44.5(3)	O(3)-Si(3)-C(13)-C(18)	71.4(6)
C(25)-Si(5)-O(11)-Cu(1)#1	-75.8(3)	O(2)-Si(3)-C(13)-C(18)	-174.3(5)
O(5)-Si(5)-O(11)-Cu(2)	-44.0(3)	O(10)-Si(4)-C(19)-C(24)	-91.4(5)
O(4)-Si(5)-O(11)-Cu(2)	-165.6(2)	O(3)-Si(4)-C(19)-C(24)	146.7(5)
C(25)-Si(5)-O(11)-Cu(2)	74.1(3)	O(4)-Si(4)-C(19)-C(24)	30.2(5)
O(6)-Si(6)-O(12)-Cu(2)	94.8(3)	O(10)-Si(4)-C(19)-C(20)	83.6(5)
O(5)-Si(6)-O(12)-Cu(2)	-26.7(4)	O(3)-Si(4)-C(19)-C(20)	-38.2(5)
C(31)-Si(6)-O(12)-Cu(2)	-147.0(3)	O(4)-Si(4)-C(19)-C(20)	-154.7(5)
O(6)-Si(6)-O(12)-Na(2)	-115.8(3)	C(24)-C(19)-C(20)-C(21)	0.9(9)
O(5)-Si(6)-O(12)-Na(2)	122.7(3)	Si(4)-C(19)-C(20)-C(21)	-174.4(5)
C(31)-Si(6)-O(12)-Na(2)	2.4(4)	C(19)-C(20)-C(21)-C(22)	-0.5(10)
O(6)-Si(6)-O(12)-Na(1)	-18.2(3)	C(20)-C(21)-C(22)-C(23)	-0.7(10)
O(5)-Si(6)-O(12)-Na(1)	-139.68(19)	C(21)-C(22)-C(23)-C(24)	1.5(10)
C(31)-Si(6)-O(12)-Na(1)	100.0(2)	C(22)-C(23)-C(24)-C(19)	-1.1(10)
C(37)-P(1)-O(13)-Na(1)	-40.9(5)	C(20)-C(19)-C(24)-C(23)	-0.1(9)
C(43)-P(1)-O(13)-Na(1)	79.2(4)	Si(4)-C(19)-C(24)-C(23)	175.2(5)
C(49)-P(1)-O(13)-Na(1)	-157.6(4)	O(11)-Si(5)-C(25)-C(30)	-127.0(5)
C(37)-P(1)-O(13)-Na(2)	144.8(3)	O(5)-Si(5)-C(25)-C(30)	-7.1(5)
C(43)-P(1)-O(13)-Na(2)	-95.2(3)	O(4)-Si(5)-C(25)-C(30)	113.2(5)
C(49)-P(1)-O(13)-Na(2)	28.0(4)	O(11)-Si(5)-C(25)-C(26)	50.9(6)
C(56)-P(2)-O(14)-Na(2)	122.2(4)	O(5)-Si(5)-C(25)-C(26)	170.8(5)
C(50)-P(2)-O(14)-Na(2)	-119.4(4)	O(4)-Si(5)-C(25)-C(26)	-68.9(5)
C(49)-P(2)-O(14)-Na(2)	0.6(5)	C(30)-C(25)-C(26)-C(27)	0.9(10)
O(7)-Si(1)-C(1)-C(2)	-2.6(5)	Si(5)-C(25)-C(26)-C(27)	-177.1(6)
O(6)-Si(1)-C(1)-C(2)	-125.1(5)	C(25)-C(26)-C(27)-C(28)	-0.1(12)
O(1)-Si(1)-C(1)-C(2)	120.6(5)	C(26)-C(27)-C(28)-C(29)	-1.0(13)
Na(1)-Si(1)-C(1)-C(2)	-41.4(5)	C(27)-C(28)-C(29)-C(30)	1.1(12)
O(7)-Si(1)-C(1)-C(6)	178.6(4)	C(28)-C(29)-C(30)-C(25)	-0.2(11)
O(6)-Si(1)-C(1)-C(6)	56.1(5)	C(26)-C(25)-C(30)-C(29)	-0.8(9)
O(1)-Si(1)-C(1)-C(6)	-58.2(5)	Si(5)-C(25)-C(30)-C(29)	177.2(5)
Na(1)-Si(1)-C(1)-C(6)	139.9(4)	O(12)-Si(6)-C(31)-C(32)	45.5(5)
C(6)-C(1)-C(2)-C(3)	1.1(9)	O(6)-Si(6)-C(31)-C(32)	169.0(4)
Si(1)-C(1)-C(2)-C(3)	-177.7(5)	O(5)-Si(6)-C(31)-C(32)	-76.4(5)
C(1)-C(2)-C(3)-C(4)	-1.3(10)	O(12)-Si(6)-C(31)-C(36)	-136.4(4)
C(2)-C(3)-C(4)-C(5)	0.7(10)	O(6)-Si(6)-C(31)-C(36)	-12.9(5)
C(3)-C(4)-C(5)-C(6)	0.0(10)	O(5)-Si(6)-C(31)-C(36)	101.7(4)
C(4)-C(5)-C(6)-C(1)	-0.2(10)	C(36)-C(31)-C(32)-C(33)	0.0(8)

Si(6)-C(31)-C(32)-C(33)	178.1(4)	C(43)-P(1)-C(49)-P(2)	70.9(4)
C(31)-C(32)-C(33)-C(34)	0.7(9)	O(14)-P(2)-C(49)-P(1)	41.3(4)
C(32)-C(33)-C(34)-C(35)	-0.7(9)	C(56)-P(2)-C(49)-P(1)	-83.2(4)
C(33)-C(34)-C(35)-C(36)	0.0(9)	C(50)-P(2)-C(49)-P(1)	165.1(3)
C(34)-C(35)-C(36)-C(31)	0.7(9)	Na(2)-P(2)-C(49)-P(1)	41.6(3)
C(32)-C(31)-C(36)-C(35)	-0.7(8)	O(14)-P(2)-C(50)-C(55)	-23.3(6)
Si(6)-C(31)-C(36)-C(35)	-178.9(5)	C(56)-P(2)-C(50)-C(55)	98.5(5)
O(13)-P(1)-C(37)-C(42)	-26.4(5)	C(49)-P(2)-C(50)-C(55)	-149.4(5)
C(43)-P(1)-C(37)-C(42)	-149.5(5)	Na(2)-P(2)-C(50)-C(55)	-52.2(6)
C(49)-P(1)-C(37)-C(42)	95.0(5)	O(14)-P(2)-C(50)-C(51)	158.1(6)
O(13)-P(1)-C(37)-C(38)	153.9(5)	C(56)-P(2)-C(50)-C(51)	-80.0(6)
C(43)-P(1)-C(37)-C(38)	30.8(6)	C(49)-P(2)-C(50)-C(51)	32.0(6)
C(49)-P(1)-C(37)-C(38)	-84.7(5)	Na(2)-P(2)-C(50)-C(51)	129.2(5)
C(42)-C(37)-C(38)-C(39)	0.2(10)	C(55)-C(50)-C(51)-C(52)	-0.5(11)
P(1)-C(37)-C(38)-C(39)	179.9(5)	P(2)-C(50)-C(51)-C(52)	178.1(6)
C(37)-C(38)-C(39)-C(40)	-0.8(11)	C(50)-C(51)-C(52)-C(53)	1.4(13)
C(38)-C(39)-C(40)-C(41)	1.0(12)	C(51)-C(52)-C(53)-C(54)	-1.3(14)
C(39)-C(40)-C(41)-C(42)	-0.5(11)	C(52)-C(53)-C(54)-C(55)	0.3(13)
C(38)-C(37)-C(42)-C(41)	0.3(9)	C(51)-C(50)-C(55)-C(54)	-0.6(10)
P(1)-C(37)-C(42)-C(41)	-179.4(5)	P(2)-C(50)-C(55)-C(54)	-179.2(6)
C(40)-C(41)-C(42)-C(37)	-0.2(10)	C(53)-C(54)-C(55)-C(50)	0.6(11)
O(13)-P(1)-C(43)-C(48)	149.6(5)	O(14)-P(2)-C(56)-C(57)	-12.5(7)
C(37)-P(1)-C(43)-C(48)	-87.5(6)	C(50)-P(2)-C(56)-C(57)	-134.6(6)
C(49)-P(1)-C(43)-C(48)	24.7(6)	C(49)-P(2)-C(56)-C(57)	114.3(6)
O(13)-P(1)-C(43)-C(44)	-32.6(6)	Na(2)-P(2)-C(56)-C(57)	15.8(7)
C(37)-P(1)-C(43)-C(44)	90.4(6)	O(14)-P(2)-C(56)-C(61)	169.7(5)
C(49)-P(1)-C(43)-C(44)	-157.4(5)	C(50)-P(2)-C(56)-C(61)	47.6(6)
C(48)-C(43)-C(44)-C(45)	-3.5(11)	C(49)-P(2)-C(56)-C(61)	-63.5(6)
P(1)-C(43)-C(44)-C(45)	178.5(7)	Na(2)-P(2)-C(56)-C(61)	-162.1(4)
C(43)-C(44)-C(45)-C(46)	0.6(14)	C(61)-C(56)-C(57)-C(58)	1.7(11)
C(44)-C(45)-C(46)-C(47)	1.5(14)	P(2)-C(56)-C(57)-C(58)	-176.2(7)
C(45)-C(46)-C(47)-C(48)	-0.6(12)	C(56)-C(57)-C(58)-C(59)	-0.5(14)
C(44)-C(43)-C(48)-C(47)	4.5(9)	C(57)-C(58)-C(59)-C(60)	-1.2(15)
P(1)-C(43)-C(48)-C(47)	-177.7(5)	C(58)-C(59)-C(60)-C(61)	1.5(13)
C(46)-C(47)-C(48)-C(43)	-2.4(10)	C(59)-C(60)-C(61)-C(56)	-0.2(11)
O(13)-P(1)-C(49)-P(2)	-54.0(4)	C(57)-C(56)-C(61)-C(60)	-1.4(10)
C(37)-P(1)-C(49)-P(2)	-175.2(3)	P(2)-C(56)-C(61)-C(60)	176.4(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+1

Table S7. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(15)-H(15O)...O(10)#1	0.91	1.90	2.762(6)	159

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+1

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